Environmental risk evaluation report: 3,3,4,4,5,5,6,6,6-Nonafluorohexene [Perfluorobutylethylene; PFBE]

(CAS no. 19430-93-4)

Chief Scientist’s Group report

April 2023

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Dr Robert Bradburne
Chief Scientist

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Executive summary

There is growing regulatory concern at international level about the emissions of per- and polyfluoroalkyl substances (PFAS) to the environment. This is due to their extreme persistence, which could lead to long-term exposure of both people and wildlife. High levels of exposure to certain PFAS has also been shown to cause harmful effects in humans and some have been declared to be 'Persistent Organic Pollutants' (POPs) under the United Nations Environment Programme (UNEP) Stockholm Convention.The UK Government is developing an action plan to address the concerns arising from PFAS. As a contribution to this work, the Environment Agency informally reviewed several PFAS that are known to be made or used at two UK production facilities. The substance reviewed in this evaluation report is 3,3,4,4,5,5,6,6,6-nonafluorohexene, also known as perfluorobutylethylene or PFBE (CAS number 19430-93-4).

PFBE is a PFAS that belongs to the group of hydrofluorocarbons. The Environment Agency has identified publicly available information on the regulatory status, uses, physico-chemical properties, environmental fate and (eco)toxicity of PFBE and has reviewed this information for reliability. Further information has also been sought from the UK importer. The data were then used to conduct an environmental hazard and risk assessment. Human health hazards have only been reviewed in so far as they are relevant for the environmental assessment. Potential risks to people following environmental exposure have not been addressed.

PFBE is not readily biodegradable, does not hydrolyse and is not expected to undergo photolysis in air. In addition, there is no information on degradation rates or half-lives available from simulation studies. PFBE is therefore considered to be potentially persistent or very persistent (P/vP). Based on screening data, PFBE is not considered to be bioaccumulative (B) in aquatic organisms. Bioaccumulation in air-breathing organisms is unlikely to be high, but there is some uncertainty in this conclusion. PFBE does not meet the criteria to be considered toxic (T). PFBE is therefore not considered to be PBT or vPvB.

Draft criteria have been proposed by the EU to identify chemicals that are persistent, mobile and toxic (PMT) or very persistent and very mobile (vPvM). PFBE does not meet the draft PMT criteria but does screen as vPvM. On the basis of low releases and lack of significant adverse effects according to the information currently available, the Environment Agency considers that the direct risk to the environment from PFBE is likely to be low. However, PFBE is expected to partition to the atmosphere and could make a contribution to global warming.

A number of recommendations are made to improve the data package to allow a more robust assessment of the environmental hazards and risks posed by PFBE. This report, along with others in this series, will be used by the Environment Agency to inform the UK Government action plan on PFAS and the PFAS Regulatory Management Options Analysis (RMOA) being conducted under the UK REACH Regulation.

Introduction

There is growing international concern about the emissions of per- and polyfluoroalkyl substances (PFAS) to the environment. This is principally due to their extreme persistence, which could lead to long-term irreversible exposure of both people and wildlife. High levels of exposure to certain PFAS has also been shown to cause harmful effects in humans and some have been declared to be ‘Persistent Organic Pollutants’ (POPs) under the United Nations Environment Programme (UNEP) Stockholm Convention.

The UK Government is developing an action plan to address the concerns arising from PFAS. As a contribution to this work, the Environment Agency informally reviewed several substances that are made or used at two known production facilities in the UK, namely AGC Chemicals Europe Ltd of Thornton Cleveleys, Lancashire and F2 Chemicals Ltd of Preston, Lancashire. Based on information provided by these companies, a provisional list of PFAS for further consideration was drawn up. This was narrowed down to the following eight substances which were, at the time, registered at more than 1 tonne per year under the EU REACH Regulation[1]. Additionally a potential substitute for perfluoroctanesulfonic acid (PFOS, which is a known POP) was included that had been identified from UK surface water monitoring. All of the substances chosen for further evaluation are listed below, initially using their EU-registered name:

- Ammonium difluoro[1,1,2,2-tetrafluoro-2-(pentafluoroethoxy)ethoxy]acetate - also known as perfluoro(2-ethoxy-2-fluoroethoxy)acetic acid ammonium salt or EEA-NH_4 (CAS no. 908020-52-0)
- Trideca-1,1,1,2,2,3,3,4,4,5,5,6,6-fluorohexane - also known as 1H-Perfluorohexane or 1H-PFHx (CAS no. 355-37-3)
- **3,3,4,4,5,5,6,6,6-Nonafluorohexene - also known as perfluorobutylethylene or PFBE (CAS no. 19430-93-4)**
- 1,1,1,2,2,3,3-Heptafluoro-3-[(trifluorovinyl)oxy]propane - also known as perfluoro(propyl vinyl ether) or PPVE (CAS no. 1623-05-8)
- 1,1,1,2,2,3,3,4,5,5,5-Undecafluoro-4-(trifluoromethyl)pentane - also known as perfluoroisohexane or PFiHx (CAS no. 355-04-4)
- Perflunafene - also known as perfluorodecalin or PFD (CAS no. 306-94-5)
- Hexafluoropropene or HFP (CAS no. 116-15-4)

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[1] Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) - see: https://ec.europa.eu/environment/chemicals/reach/reach_en.htm

- Octafluoropropane - also known as perfluoropropane or PFP (CAS no. 76-19-7)

The additional substance also being considered is:

- 6:2 Chlorinated polyfluorinated ether sulfonate - also known as 'F-53B' (CAS no. 73606-19-6)

This report summarises the evaluation of the substance highlighted above in **bold** (i.e. PFBE), to address the following questions:

- What data are currently available, and are they sufficiently reliable to assess the environmental hazards and risks from this substance?
- Can we establish numerical exposure limits for assessing environmental impacts (e.g. for use under permitting regimes)?
- Is this substance potentially able to reach remote environments and what is its groundwater contamination potential?
- Is this substance a potential candidate for future risk management?
- What information gaps remain, relative to the registered tonnage of this substance and, if required, what is the most appropriate way of obtaining this information?

The Environment Agency has performed a literature review (Appendix A). Information on the substance's properties and uses is also provided on the European Chemicals Agency (ECHA) public dissemination website (ECHA, 2020). Unless stated otherwise, this website and data provided by the UK importer are the main source of the information for this report. Full scientific study reports have generally not been reviewed by the Environment Agency, only the publicly available literature and EU REACH dossier information have been consulted at this stage.

This report describes the substance and its structural analogues, its analytical chemistry, manufacture and use, regulatory status and then various environmentally relevant properties. This is followed by an environmental hazard assessment in Section 9, and an exposure and risk assessment in Sections 10 and 11. The final section (Section 12) summarises our findings. Although the focus of this evaluation is on environmental hazards and risks, there is a brief summary of mammalian toxicology information, where available and relevant. However, this report is not intended to provide a full consideration of hazards, exposure and risks to human health. This is not a formal UK REACH evaluation.

1 Substance identity

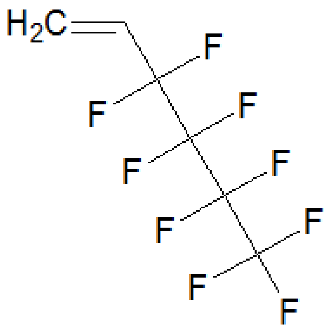
1.1 Name and other identifiers

Table 1.1 Substance identifiers

Public name	3,3,4,4,5,5,6,6,6-nonafluorohexene
IUPAC name	3,3,4,4,5,5,6,6,6-nonafluorohex-1-ene
CAS name	Perfluorobutyl(ethylene)
EC number	243-053-7
CAS number	19430-9-34
Index number in Annex VI of the CLP Regulation	Not applicable
Molecular formula	$C_6H_3F_9$
Molecular weight	246.07 g/mol
SMILES code	C=CC(C(C(C(F)(F)F)(F)F)(F)F)(F)F
Synonyms	(Perfluorobutyl)ethylene ; 3,3,4,4,5,5,6,6,6-Nonafluoro-1-hexene ; Perfluorobutylethylene ; 1H,1H,2H-Perfluoro-1-hexene ; 3,3,4,4,5,5,6,6,6-nonafluorohex-1-ene ; 1h,1h,2h-perfluorohexene ; (Perfluorobutyl)ethene ; 1-Hexene, 3,3,4,4,5,5,6,6,6-nonafluoro- ; 3,3,4,4,5,5,6,6,6-Nonafluorohexene ; (Perfluoro-n-butyl)ethylene ; perfluorobutyl ethylene ; 1h,1h,2h-perfluorohex-1-ene ; Nonafluorobutylethene ; 1h,1h,2h-nonafluorohex-1-ene ; Zonyl(R) PFBE fluorotelomer intermediate ; 3,3,4,4,5,5,6,6,6-Nonafluoro-1-hexene ; 3,3,4,4,5,5,6,6,6-nonakis(fluoranyl)hex-1-ene ; MP7360000 ; PFBE
Type of substance	mono-constituent

SMILES - Simplified Molecular Input Line Entry System

Figure 1.1 Structural formula of PFBE representing the atoms and how they are bonded to each other



The substance is called PFBE throughout this report.

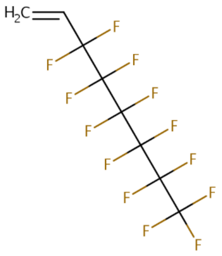
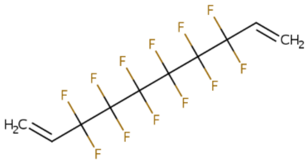
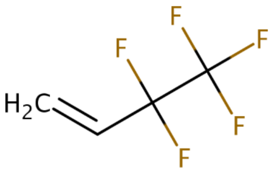
1.2 Structurally related substances

PFBE has a perfluorinated chain of 4 carbon atoms with a non-fluorinated ethene group at one end of the chain. It is an example of a hydrofluorocarbon (HFC).

Structurally related substances to PFBE were identified through the US Environmental Protection Agency (US EPA) CompTox Dashboard (US EPA, 2022a) and the PubChem Dashboard (NCBI, 2022). The dashboards identify related substances in their records using connectivity (first layer 'InChI'), mixture components and isotopic isomers, and the Tanimoto coefficient (>0.8). InChI is the IUPAC international identifier, and uses a software model to assign an identifier to a molecule which describes structure. The dashboards suggested 99 structural analogues, tabulated in Appendix B.

Only 3 of the 99 substances have been subject to registration under EU REACH. The Environment Agency therefore selected these as suitable structural analogues for PFBE, based on chemical similarity (Tanimoto coefficient >0.8) and the availability of relevant data. They are listed in Table 1.2. These analogues have slightly shorter or longer carbon chains with similar structural features to PFBE, and so provide additional context to support conclusions about the behaviour of this type of substance.

Table 1.2 Substance identifiers for selected analogues of PFBE

Name	**Tridecafluorooctene**	**1,6-Divinyl-perfluorohexane**	**3,3,4,4,4-Pentafluorobut-1-ene**
CAS number	25291-17-2	1800-91-5	374-27-6
EC number	246-791-8	217-288-0	206-775-3
Structural formula			
Molecular formula	$C_8H_3F_{13}$	$C_{10}H_6F_{12}$	$C_4H_3F_5$
Molecular weight	346.09 g/mol	354.14 g/mol	146.06 g/mol
SMILES code	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=C	FC(F)(C=C)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=C	FC(F)(F)C(F)(F)C=C
Synonyms	3,3,4,4,5,5,6,67,7,8,8,8-Tridecafluorooct-1-ene	3,3,4,4,5,5,6,6,7,7,8,8-Dodecafluorodeca-1,9-diene	-
Comment	Differs from PFBE only in the length of the fluorinated carbon chain, with 2 additional fluorinated carbon atoms.	Differs from PFBE in having 2 terminal ethene groups and 2 additional fluorinated carbon atoms.	Differs from PFBE only in the length of the fluorinated carbon chain, with 2 fewer fluorinated carbon atoms.
Reference	ECHA, 2022d US EPA, 2022c	ECHA, 2022c US EPA, 2022n	ECHA, 2022e US EPA, 2022ck

1.3 Transformation products

There is no information relating to identified or predicted transformation products of PFBE in the REACH registration. Although the carbon-fluorine bond is very strong, a slow reaction occurred in the ready biodegradation test (Section 6). The transformation products were not identified but could be shorter perfluorinated chains following removal of the ethene group, either perfluoropentanoic acid or perfluorobutanoic acid. These would be expected to be highly resistant to further transformation.

2 Analytical chemistry

2.1 Regulatory and academic methods

The EU registration dossier does not provide any analytical details (ECHA, 2022a).

The Environment Agency searched the academic literature for analytical methods for the detection of PFBE in environmental matrices (water, fresh and marine; soil, sediment, sludge and air). Numerous methods relating to short chain perfluorocarbons (PFCs) were found, although no specific methods for PFBE were identified.

Analytical monitoring of PFBE in environmental matrices is not documented as part of national or international monitoring programmes. It is, however, present in databases operated by the Swedish Chemicals Agency, OECD Global Database, EPA ToxCast/Tox21 and several others. No validated associated analytical methods were presented alongside. The US EPA states that methods for measurement of volatile PFAS in air are under development and undergoing validation (US EPA, 2022da).

The website of the contract laboratory Eurofins Test America (www.EurofinsUS.com/PFAS) indicates they have a validated method for the quantification of volatile perfluoroalkyl carboxylic acids in air. This method may be adaptable to allow measurement of PFBE.

The Environment Agency considers that the description of a robust analytical method will typically include the following details:

- Instruments and consumables including chromatographic column, temperature, mobile phase composition, flow rates, gradient or isocratic separation and the detector optimisation and configuration.
- Certified reference standards, calibration range and sensitivity, limit of detection, limit of quantification, column recoveries, stability and reproducibility.
- Sample preparation including clean-up consumables, concentration techniques and use of internal standards (plus justification for choice) for validation and recoveries, etc.
- Identification and discussion of technical limitations.

3 Import, manufacture and uses

Although the UK left the European Union (EU) at the end of January 2020, European legislation in place by December 2020 has been retained and transposed into UK law, and ECHA is still the most relevant source of information about chemicals on the UK market at the time of writing.

PFBE is registered under the EU REACH Regulation at a supply level of 100 to 1 000 tonnes/year. There are two EU REACH Registrants, AGC Chemicals Europe Ltd (www.agcce.com) and Chemours Netherlands B.V. (both located in the Netherlands). There is a single grandfathered registration under UK REACH also at a supply level of 100 to 1 000 tonnes/year.

The substance is imported into the UK for use at AGC Chemicals Europe Ltd's manufacturing site at Thornton Cleveleys near Blackpool, Lancashire. AGC Chemicals Europe Ltd has an environmental permit (ref: EPR/BU5453IY) under the Environmental Permitting (England and Wales) Regulations 2016. It produces two main product streams:

- polytetrafluoroethylene (PTFE) with a capacity up to 4 000 tonnes/year
- ethylene-tetrafluoroethylene (ETFE) with a capacity up to 2 000 tonnes/year

PFBE is used as a co-monomer to manufacture PTFE and ETFE. AGC Chemicals Europe Ltd has informed the Environment Agency that their polymer products are used in many applications including for wire coatings, cables and tubing in the semi-conductor industry and cable insulation in the automotive and aerospace industry.

An overview of uses provided in the EU REACH registration information on the ECHA website is presented in Table 3.1.

Table 3.1 Overview of uses

Life cycle stage	Use(s)
Uses at industrial sites	ERC6a: Use of intermediate ERC 6c: Use as a monomer in polymerisation process PROC 1: Chemical production or refinery in closed process without likelihood of exposure or processes with equivalent containment conditions PROC 2: Chemical production or refinery in closed continuous process with occasional controlled exposure or processes with equivalent containment conditions PROC 3: Manufacture or formulation in the chemical industry in closed batch processes with occasional controlled exposure or processes with equivalent containment conditions PROC 8b: Transfer of substance or mixture (charging and discharging) at dedicated facilities PROC 15: Use as laboratory reagent
Uses by professional workers	None identified in registration dossier
Consumer Uses	None identified in registration dossier
Article service life	None identified in registration dossier

Note: PROC codes are Process Codes, which describe process types.

4 Summary of relevant regulatory activities

4.1 Europe

4.1.1 European Chemicals Agency (ECHA)

The Public Activities Co-ordination Tool (PACT) (https://echa.europa.eu/pact accessed March 2022) provides an overview of the substance-specific activities that EU regulatory authorities are working on under the EU REACH and CLP Regulations. To date the only substance-specific activities identified for PFBE are dossier evaluation and a testing proposal for a sub-chronic toxicity study (90 days) (inhalation) according to OECD Test Guideline (TG) 413 in the rat (OECD, 2018b), which was concluded on 11 January 2016.

Between May and July 2020, the national authorities of Germany, the Netherlands, Norway, Sweden and Denmark invited interested parties to send in evidence and information on the use of PFAS in preparation for a joint EU REACH restriction proposal. The current scope of the work is wide and includes all substances that contain at least one aliphatic -CF2- or -CF3 element (see ECHA Registry of Restriction Intentions: https://echa.europa.eu/registry-of-restriction-intentions/-/dislist/details/0b0236e18663449b, accessed March 2022). PFBE is therefore within scope of this initiative.

4.1.2 European Food Safety Agency (EFSA)

EFSA provides scientific advice on safety of food additives, enzymes, flavourings, processing aids and other substances intentionally added to food; safety of food packing and other food contact materials.

A search of the EFSA website (http://www.efsa.europa.eu/) identified PFBE as noted under three published scientific opinions.

These were:

- Scientific opinion on the safety evaluation of the substance, (perfluorobutyl)ethylene, CAS No. 19430-93-4, for use in food contact materials (February 2011)
- 62nd plenary meeting of the European Food Safety Authority (EFSA) panel on food contact materials, enzymes, flavourings and processing aids (CEF), request for the re-evaluation of PFBE (June 2016)
- 5th plenary meeting of the EFSA panel on food contact materials, enzymes and processing aids (CEP) panel, request for the re-evaluation of PFBE (February 2019)

4.1.3 Oslo and Paris Convention for the Protection of the Marine Environment of the North-East Atlantic (OSPAR)

The Oslo and Paris Convention for the Protection of the Marine Environment of the North-East Atlantic (OSPAR) is a mechanism by which 15 national governments and the EU co-operate to protect marine resources. Much of OSPAR's work on chemicals is now being addressed by REACH activities.

PFBE is not on the OSPAR List of Substances of Possible Concern (www.ospar.org/work-areas/hasec/chemicals/possible-concern/list, accessed March 2022). PFBE is also not on the list of Chemicals for Priority Action adopted in 2002 (www.ospar.org/work-areas/hasec/chemicals/priority-action, accessed March 2022).

4.2 Regulatory activity outside Europe

4.2.1 United States

PFBE is listed as one of the substances undergoing risk evaluation as part of US EPA's existing chemical initiative under the Toxic Substances Control Act (TSCA) to determine whether they present an unreasonable risk to public health or the environment under the conditions of use (US EPA, 2022).

4.2.2 Canada

A search did not identify PFBE as being under assessment under the Prohibition of Certain Toxic Substances Regulations, 2012 (https://www.canada.ca/en/environment-climate-change/services/canadian-environmental-protection-act-registry/substances-list/toxic.html, accessed March 2022).

4.2.3 Australia

A search did not identify PFBE as being under assessment under the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) (https://www.nicnas.gov.au/chemical-information/imap-assessments/imap-assessments, accessed March 2022), or on the list of chemicals with high hazard (https://www.industrialchemicals.gov.au/help-and-guides/list-chemicals-high-hazards-categorisation) accessed March 2022).

4.2.4 New Zealand

A search did not identify PFBE as being under assessment under the Hazardous Substances and New Organisms Act 1996 (https://www.epa.govt.nz/industry-areas/hazardous-substances/, accessed March 2022; https://www.epa.govt.nz/industry-areas/hazardous-substances/chemical-reassessment-programme/screened-chemicals-list/, accessed March 2022).

4.2.5 Japan

Industrial chemicals are managed under the Chemical Substances Control Law (CSCL), most recently amended in 2009 (https://www.nite.go.jp/chem/jcheck/list3.action?category=141&request_locale=en, accessed March 2022). Under the Act there are 3 lists:

- Class I Specified Chemicals - 34 substances (persistent, bioaccumulative, toxic)
- Class II Specified Chemicals - 23 substances (toxic and high risk)
- Priority Assessment Chemical Substance (PACS), currently 227 substances

PFBE is not on any of the above lists.

4.3 Other international agreements

4.3.1 United Nations Stockholm Convention on Persistent Organic Pollutants (POPs)

PFBE is not identified as a POP, and is not currently under evaluation (http://chm.pops.int/TheConvention/ThePOPs/AllPOPs/tabid/2509/Default.aspx, accessed March 2022).

4.3.2 Greenhouse gases

Although not a gas, PFBE is a volatile liquid and environmental exposure is therefore likely to result in atmospheric exposure.

Fluorinated gases (‘F-gases’) may contribute to climate change due to their global warming potential and they are often used as substitutes for ozone-depleting substances, because they do not damage the atmospheric ozone layer (EC, n.d.). F-gases are regulated under the Ozone-Depleting Substances and Fluorinated Greenhouse Gases (Amendment etc.) (EU Exit) Regulations (2019) which aims to reduce the emission of these gases into the environment. Annex I and II list the F-gases subject to the Regulation and PFBE is not included.

5 Physicochemical properties

This evaluation focusses on vapour pressure, water solubility and n-octanol/water partition coefficient, as they are the key physicochemical end points for the environmental assessment of most organic chemicals. Surface tension and dissociation constant are also considered. The available information is discussed in this section, and a conclusion drawn about which value the Environment Agency considers most suitable for the further evaluation of this substance.

The source of this information is the publicly available EU REACH registration database (ECHA, 2022a; accessed March 2022) unless otherwise indicated. The reliability scores provided in the full registration for individual studies are cited. These scores have presumably been generated in accordance with the ECHA R.4. Guidance Document (ECHA, 2011).

The Environment Agency has not evaluated original study reports. Where an independent evaluation has not been possible for a study, or the EU REACH registration dossiers lack sufficient supporting information, this is noted in the text (except in the case of data presented in academic journals or obtained using quantitative structure-activity relationship (QSAR) models).

Where an endpoint value is missing from the EU REACH registration dossier, or an initial review raised questions around the validity of an experimentally derived value, the assessment has been supplemented with information from analogues (see Section 1) and openly available *in silico* QSAR models. REACH registration data for the analogues are taken at face value, although preference is given to regulatory reviews (if available). QSAR models are generally considered to be a screening-level tool and measured values are preferable provided that they are sufficiently reliable. Further information is provided in Appendix C.

An overview of physicochemical data provided in the EU registration dossier or generated by the Environment Agency is presented in Table 5.1.

Table 5.1 Summary of physicochemical properties for PFBE

Property	Value(s)	Reliability	Source
Physical state at 20 °C and 101.3 kPa	Clear colourless liquid with an ether like odour	Registrant: 2 (key study)	EU REACH Registration dossier
Melting / freezing point	<-20°C at 101.3kPa (GLP, EU Method A.1)	Registrant: 1 (key study)	EU REACH Registration dossier
Boiling point	58°C at 101.3kPa (ACGIH handbook)	Registrant: 2 (key study)	EU REACH Registration dossier
Relative density	1 400 g/L (1.4 g/cm^3 at 20 °C (ACGIH handbook)	Registrant: 2 (key study)	EU REACH Registration dossier
Vapour pressure	22 kPa at 20 °C (167 mmHg) (Du Pont study)	Registrant: 2 (key study)	EU REACH Registration dossier
Surface tension	Data waiver	n/a	EU REACH Registration dossier
Water solubility	15.6 mg/L at 20 °C and pH 7 (GLP, OECD TG 105)	Registrant: 1 (key study)	EU REACH Registration dossier
n-Octanol/water partition coefficient (log K_{OW})	4.13 at 25 °C and pH 7.4 (GLP, OECD TG 117)	Registrant: 1 (key study)	EU REACH Registration dossier
n-Octanol/air partition coefficient (log K_{OA})	0.47 (KOAWIN v1.10 estimate, EPISuite™, Log K_{ow} used 4.99)	Environment Agency: n/a	Environment Agency
Dissociation constant	Not applicable	-	-

5.1 Vapour pressure

5.1.1 Measured data

The reported vapour pressure of PFBE in the EU REACH registration dossier was 22 kPa at 20 °C (ECHA, 2022a). This key experimental study was not performed according to an accepted test guideline. No further details on the method were provided, although the EU registration dossier rates it reliable with restrictions (Klimisch 2). The Environment Agency has been unable to review the full study report and therefore cannot comment on its reliability.

An additional experimentally derived vapour pressure of 31.7 kPa at 20 °C is available on the PubChem database (NCBI, 2022), acquired from NIOSH 2008. The reliability of this result is unknown.

5.1.2 Predicted data

No *in silico* predictive data were presented in the EU registration dossier for this endpoint as there is an experimental result.

For comparative purposes, the Environment Agency has considered readily available QSARs to test how they perform for this type of substance. The ChemSpider database and the US EPA CompTox dashboard contain predicted vapour pressures for PFBE generated from EPISuite^{TM} v4.0 (T.E.S.T.), ACD/Labs and OPERA software (RSC, 2022; US EPA, 2022a). Median predicted values are presented in Table 5.2. The Environment Agency converted the values from mmHg to kPa.

Table 5.2 Predicted vapour pressures for PFBE

Source	Prediction method	Predicted vapour pressure (kPa/mmHg) at 25 °C
ACD/Labs (US EPA 2022a)	Not available	44.26 kPa 332 mmHg
ACD/Labs (RSC 2022)	Not available	44.32 kPa 332.4 mmHg
EPISuite™ Estimation programme MPBPWIN v 1.42 (RSC 2022)	Mean of Antoine and Grain methods BP = 7.79 °C MP = -105.83 °C	183.98 kPa 1 380 mmHg
T.E.S.T. (EPISuite™ v 4.00) (US EPA 2022a)	Not available	55.86 kPa 419 mmHg
OPERA (US EPA 2022a)	Not available	285.31 kPa 2.14 × 10^3 mmHg

In silico predicted values should always be treated with caution where substances in the training set and external test set are not visible. For the ACD/Labs and MPBPWIN models this information was not available. Therefore, no assessment of applicability could be performed. The good agreement between predicted and measured value using the ACD/Labs model may be coincidental.

Structural analogues of PFBE were included in both the training set and external test sets for the T.E.S.T. and OPERA models. Predicted vapour pressure values could therefore be within the applicability domain of both models, although this was not clear. Despite this, there is a large difference between the predicted and experimental values, illustrating the difficulty in prediction of properties of PFAS and that the OPERA model in particular is not reliable in this case.

5.1.3 Data from structural analogues

Experimentally derived vapour pressures were presented for two of the selected structural analogues of PFBE, namely:

- 3,3,4,4,5,5,6,6,7,7,8,8-dodecafluorodeca-1,9-diene: 1 200 Pa (1.2 kPa) at 20 °C and 1 900 Pa (1.9 kPa) at 25 °C (ECHA, 2022c; US EPA, 2022n)
- 3,3,4,4,4-pentafluorobut-1-ene: 1.9 to 2.1×10^5 Pa (190 to 210 kPa) at 25 °C (ECHA, 2022e; US EPA, 2022ck)

5.1.4 Additional sources

Due to the availability of experimentally derived values for vapour pressure for PFBE as well as two of its structural analogues no additional sources were consulted.

5.1.5 Recommended value

An experimental vapour pressure value of 22 kPa at 20 °C was reported for PFBE in the EU registration dossier (ECHA, 2022a). Furthermore, a similar experimentally derived vapour pressure (31.7 kPa at 20 °C) has been reported separately (NCBI, 2022). Neither of these values were accompanied by adequate supporting information to allow an assessment of reliability.

In silico predicted values range from 44.26 kPa to 285.31 kPa (both at 25 °C; US EPA, 2022a and NCBI, 2022). There is large variation between predicted and measured values even with temperature taken into account, and the Environment Agency does not consider any of these predicted values to be reliable.

Vapour pressures for two of the selected structural analogues were available. These were 1.2 kPa at 20 °C for 3,3,4,4,5,5,6,6,7,7,8,8-dodecafluorodeca-1,9-diene, and between 19 and 21 kPa at 25 °C for 3,3,4,4,4-pentafluorobut-1-ene. The vapour pressure for PFBE would be expected to lie between these two values, because it is intermediate in terms of molecular size. Assuming that the analogue data are reliable (which has not been checked), this could suggest that the measured vapour pressures for PFBE are over-estimated.

The Environment Agency assumes that the vapour pressure of PFBE is likely to be around **22 kPa at 20 °C**, and this value is taken forward for this evaluation because it is reasonably consistent with an apparently independent measurement available on the PubChem database.

5.2 Surface tension

5.2.1 Measured data

The EU REACH registration dossier waives this endpoint based on the structure of PFBE. No data for the surface tension of PFBE could be found in the literature.

5.2.2 Predicted data

No predicted data for surface tension were provided in the EU registration dossier.

The US EPA CompTox dashboard presents predicted surface tension endpoint values for PFBE generated from T.E.S.T. and ACD/Labs software (US EPA, 2022a). These were 11 mN/m and 12.9 mN/m, respectively.

The ChemSpider database also contains a predicted surface tension of 12.9±3 dyne/cm [mN/m] performed using ACD/Labs software (RSC, 2022).

In silico predicted values should always be treated with caution where substances in the training set and external test set are not visible. For the T.E.S.T. model structural analogues of PFBE were included in the training set and external test sets (US EPA, 2022a). This information was not available for the ACD/Labs models.

5.2.3 Data from structural analogues

No data on surface tension were presented for any of the three structural analogues of PFBE.

5.2.4 Recommended value

No experimental data for the surface tension of PFBE was in the registration dossier, nor were any to be found in the literature.

The Environment Agency considers that *in silico* predicted values of surface tension for PFCs relate to the neat substance rather than that of an aqueous solution and so are not relevant for this evaluation.

Surface tension in water is important because it affects the measurement and interpretation of other physico-chemical properties such as water solubility and partition coefficients. The Environment Agency notes that PFBE does not have any hydrophilic structural groups that can form hydrogen or Van der Waals bonds in water. This suggests that it is unlikely to be significantly surface active in aqueous solutions.

5.3 Water solubility

5.3.1 Measured data

The EU REACH registration dossier summarises a water solubility value of 15.6 mg/L at 20 °C and pH 7, measured using a shake flask method in accordance with OECD TG 105 (OECD, 1995a; ECHA, 2022a). The reference, deemed GLP compliant, is dated 2001 but is not named. Water solubility was assessed across 4 flasks with measurements taken at day 4, 6, 8 and 12, ranging from 11.50 mg/L to 249.56 mg/L. All of the high values originated from one vessel and these data were excluded as outliers. The EU registration dossier consider the data reliable without restrictions (Klimisch score 1).

The Environment Agency notes that there were variations in the measured concentrations. From the EU registration dossier summary it is unclear whether any amendment to the study design was made to take into account the volatility of PFBE, which could have contributed to the observed variations. Other types of PFAS have the potential to form micelles in water, and it is not known whether this is the case for PFBE.

5.3.2 Predicted data

No *in silico* predictive data were presented in the EU registration dossier for this endpoint as there is an experimental result.

For comparative purposes, the Environment Agency has considered readily available QSAR software to test how they perform for this type of substance. The ChemSpider database and US EPA CompTox dashboard contained predicted water solubility endpoint values generated from EPISuite™, in addition, the CompTox database also included data from T.E.S.T. and OPERA software (RSC, 2022; US EPA, 2022a). These values are presented in Table 5.3. Values were converted by the Environment Agency from mol/L to mg/L using a molecular weight of 246.07 g/mol.

Table 5.3 Predicted water solubility values for PFBE

Model	Details	Water solubility
EPISuite™ water solubility estimate from log K_{ow} (WSKOW v1.41)	-	1.36 mg/L at 25 °C
EPISuite™ water solubility estimate from fragments (WATERNT v1.01 est.)	-	0.15 mg/L

T.E.S.T. **(EPISuite™ v 4.00)**	Predicted value: 7.23×10^{-6} mol/L Reasonable confidence, low mean absolute error	27.31 mg/L
OPERA	Predicted value: 3.04×10^{-5} mol/L Global applicability domain: outside Local Applicability domain index: 0.491 Confidence Interval 0.572	22.40 mg/L

In silico predicted values should always be treated with caution where substances in the training set and external test set are not visible.

- Guidance provided with the WSKOWWIN model indicates that the relationship between the experimental and predicted values for a training set of 1 450 compounds was good, with a correlation coefficient (R^2) of 0.97, standard deviation of 0.409 and an average deviation of 0.313. The validation set contained several PFCs (see Appendix C) and it is likely that the predicted value for PFBE falls within the applicability domain of the model.
- Guidance provided with the WATERNT model indicates that the relationship between the experimental and predicted values for a training set of 4 636 compounds was good, with an R^2 of 0.85, standard deviation of 1.045 and an average deviation of 0.796. The validation set contained several PFCs (see Appendix C) and it is likely that the predicted value for PFBE falls within the applicability domain of the model.
- Data generated by T.E.S.T model for PFBE were assessed as having reasonable confidence with low mean absolute error. Two analogues with reasonable Tanimoto similarity (>0.80) are included in the training set. These data should still be considered with caution.
- Structural analogues of PFBE were not included in the training set for the OPERA model. A low global applicability domain score is also given, so the prediction should therefore not be considered reliable.

The *in silico* predictions therefore suggest that the water solubility of PFBE may lie in the range 0.15 to 27.3 mg/L.

5.3.3 Data from structural analogues

Experimentally derived water solubility were presented for two of the selected structural analogues of PFBE, namely:

- 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooct-1-ene: 1.21 mg/L at 25 °C and pH 6 (ECHA, 2022d; US EPA, 2022c).

- 3,3,4,4,5,5,6,6,7,7,8,8-dodecafluorodeca-1,9-diene: 1.61 mg/L at 20 °C and at pH 5.5 (ECHA, 2022c; US EPA, 2022n).

These data have not been evaluated by the Environment Agency, so it is not known if steps were taken to address volatility.

5.3.4 Recommended value

A water solubility of 15.6 mg/L at 20 °C is reported for PFBE from a modern experimental study, which the EU registration dossier considers to be fully reliable. Variations in concentrations were noted between vessels in the study, which were excluded from the results. The influence of micelle formation and volatility is unclear, so the Environment Agency suggests that the study may be reliable with restrictions (Klimisch 2), subject to receipt of a full study report.

Predicted values of water solubility ranged from 0.15 to 27.3 mg/L.

Water solubility measurements for two of the selected structural analogues were 1.21 mg/L at 25 °C for 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooct-1-ene, and 1.61 mg/L at 20 °C for 3,3,4,4,5,5,6,6,7,7,8,8-dodecafluorodeca-1,9-diene. The solubility of PFBE would be expected to be somewhat higher than these two values, because it has a smaller molecular size, so the reported value is consistent.

The Environment considers that the water solubility of **15.6 mg/L at 20 °C** is a suitable estimate for the purposes of this evaluation.

5.4 Partition co-efficient (n-octanol/water; log K_{OW})

5.4.1 Measured data

The key experimental study for n-octanol/water dissociation constant in the EU REACH registration dossier was carried out according to OECD TG 117 (OECD, 2004) (high performance liquid chromatography (HPLC) method) and was GLP compliant (ECHA, 2022a). A log K_{OW} value of 4.13 at 25 °C and pH 7.4 was measured.

The test material was Zonyl® PFBE provided at 96% purity and the reference substances were formamide, naphthalene, phenanthrene, fluoranthene, perylene, dibenz(ah)anthracene and benzo(ghi)perylene. Three repeats and the mean of the three were presented for each chemical. Experimental retention times from triplicate measurements were consistent. OECD TG 117 states that the method is suitable for chemicals with a log K_{OW} in the range 0 to 6 and that retention times should be measured in duplicate. The EU registration dossier met these requirements. Little further information was given relating to the specific HPLC methodology. The EU registration dossier consider the data to be reliable without restrictions (Klimisch 1), and the Environment Agency agrees that the study appears to have been well performed.

The Chemspider database (RSC, 2022) contains an experimental log K_{ow} for PFBE of 4.5 but provides no further details about the method used. Therefore the reliability of this value is unknown (Klimisch 4).

As noted in Section 5.3.4, PFAS may form colloids in water. It is possible that the same may occur in organic liquids like n-octanol. The reliability of a measured K_{OW} is therefore uncertain.

5.4.2 Predicted data

No predicted data for log K_{OW} were presented in the EU registration dossier.

For comparative purposes, the Environment Agency has considered readily available QSAR software to test how they perform for this type of substance. The US EPA CompTox dashboard and ChemSpider database contained estimated log K_{OW} values for PFBE from ACD/Labs, ACD/Labs consensus, EPISuite™ and OPERA (RSC, 2022; US EPA, 2022a) (Table 5.4).

Table 5.4 Predicted log K_{OW} values for PFBE

Model	Details	log K_{OW}
ACD/Labs **Chemspider**	ACD/LogP ACD/LogD (pH 5.5) ACD/LogD (pH 7.4)	4.15 3.71 3.71
EPISuite™ **Chemspider & CompTox**	KOWWIN v 1.67 estimate	4.99
ACD/Labs **CompTox**	-	4.15
ACD/Labs Consensus **CompTox**	-	3.71
OPERA	Global applicability domain: Inside Local Applicability domain index: 0.472 Confidence Interval 0.482	3.00

In silico predicted values should always be treated with caution where substances in the training set and external test set are not visible.

- This information was not available for the ACD/labs model, so no assessment of the applicability can be performed.
- Guidance provided with the KOWWIN model indicates that the relationship between the experimental and predicted values for a validation set of 10 331 compounds was good, with an R^2 of 0.94 and standard deviation of 0.47. The training set contained several PFCs (see Appendix C) and it is likely that the predicted value for PFBE falls within the applicability domain of the model.
- For the OPERA model, PFBE is considered inside the global applicability domain and has a local applicability domain index of 0.472. The predicted value therefore has moderate confidence.

The *in silico* predictions therefore suggest that the log K_{OW} of PFBE may lie in the range 3.0 to 4.99. The model which predicts the closest value to the measured log K_{OW} is ACD/Labs, but the reliability of this model for this type of substance is unknown and so it may just be coincidence.

5.4.3 Data from structural analogues

Log K_{OW} values of 5.2 and 4.9 have been determined for 3,3,4,4,5,5,6,67,7,8,8-dodecafluorodeca-1,9-diene and 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooct-1-ene, respectively (US EPA, 2022c; US EPA, 2022n; ECHA, 2022c; ECHA, 2022d). The Environment Agency has not evaluated the reliability of these values, but it suggests that this type of substance may have a high affinity for organic phases such as lipids.

5.4.4 Recommended value

The key log K_{OW} value for PFBE provided in the EU registration dossier was 4.13 (ECHA, 2022a). This value was measured in a study performed according to OECD TG 117 and was GLP compliant. The EU registration dossier assigned a reliability score of Klimisch 1 (reliable without restriction). An apparently independent measured log K_{OW} value of 4.5 is also available on the ChemSpider database, without supporting data or information (RSC, 2022).

Several predicted log K_{OW} values for PFBE were acquired from Chemspider (RSC, 2022) and US EPA Comptox (US EPA, 2022a), ranging ranged from 3.00-4.99. The methods appear to be reasonably reliable for this type of compound.

Measured log K_{OW} values of 5.2 and 4.9 have been determined for 3,3,4,4,5,5,6,67,7,8,8-dodecafluorodeca-1,9-diene and 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooct-1-ene, respectively. These substances have a higher molecular weight than PFBE, so solubility in water and n-octanol may differ. Nevertheless, these values suggest that this type of substance may have a high affinity for organic phases such as lipids.

The Environment Agency considers that the **log K_{OW} 4.13 (at 25 °C)** presented in the EU registration dossier should be taken forward for this evaluation.

5.5 n-Octanol/air partition coefficient (log K_{OA})

The octanol-air partition coefficient is non-standard endpoint for hazard assessment under REACH. It is used to predict the partitioning behaviour of organic compounds between air and environmental matrices such as soil, vegetation, and aerosol particles (Meylan and Howard, 2005). Methods for measurement and calculation of the value are discussed in Environment Agency (2009).

5.5.1 Measured Data

No experimental log K_{OA} values were presented for PFBE in the EU registration dossier (ECHA, 2022a).

5.5.2 Predicted data

There are no predicted data for log K_{OA} in the EU REACH registration dossier.

The Environment Agency has estimated a K_{OA} value using the dimensionless Henry's Law constant (log K_{AW}) of 2.17 (see Section 6.2.4) and the recommended log K_{OW} value of 4.13 (Section 5.4) ($K_{OA} = K_{OW}/K_{AW}$). The resulting log K_{OA} is 1.96. As there is uncertainty in the K_{AW}, the reliability of the derived K_{OA} value is unknown

The US EPA CompTox dashboard and ChemSpider database contained predicted K_{OA} values for PFBE generated from KOAWIN v1.10 and OPERA software (RSC, 2022, US EPA, 2022a). These values are presented in Table 5.5.

Table 5.5 Predicted log K_{OA} for PFBE

Source	Details	log K_{OA}
EPISuite™ Estimation programme KOAWIN v1.1	Log K_{OA} (log K_{OW} used: 4.13 and log K_{AW} used: 3.657 estimated) Log K_{OA}	0.47 (Environment Agency) 1.33 (ChemSpider; RSC, 2022)
OPERA **CompTox**	Global applicability domain: Inside Local Applicability domain index: 0.973 Confidence Interval: 0.781	1.60

Calculation	Calculated from log K_{AW} of 2.17 and a log K_{OW} value of 4.13 ($K_{OA} = K_{OW}/K_{AW}$)	1.96

In silico predicted values should always be treated with caution where substances in the training set and external test set are not visible.

- For the KOAWIN model, the values for log K_{OW} presented in the EU registration dossier were used with the predicted log K_{AW} value (EPIsuite^{TM} v4.11). The training sets for KOWWIN and HENRYWIN contain several PFCs (see Appendix C) and it is likely the predicted value for PFBE falls within the applicability domains of the two models. Therefore, the predicted K_{OA} for PFBE can be considered to be predicted with reasonable confidence.
- PFBE is considered inside the global applicability domain of the OPERA model and has a high local applicability domain index (> 0.6; 0.973), so the prediction has high confidence.

5.5.3 Data from structural analogues

A calculated log K_{OA} of 2.15 was presented in the EU REACH registration of 3,3,4,4,5,5,6,6,7,7,8,8-dodecafluorodeca-1,9-diene (ECHA 2022c). However, the Environment Agency considers that the Henry's Law constant used to calculate the value may be incorrect, so it is not considered further.

5.5.4 Recommended value

In silico predictions for the log K_{OA} of PFBE are between 0.47 and 1.60, depending on the input parameters and models used.

The Environment Agency has estimated a log K_{OA} is 1.96 from the dimensionless Henry's Law constant and recommended log K_{OW} value, although there may be some uncertainty in this value.

Overall, the Environment Agency considers that the log K_{OA} likely falls in the range of 0.47 to 1.96, although there are uncertainties. A value of **1.0** is therefore suggested for the purposes of this evaluation.

5.6 Dissociation constant

No experimental dissociation constants were presented for PFBE in the EU registration dossier (ECHA, 2022a). The Environment Agency notes that a dissociation constant is irrelevant for PFBE as it has no ionisable functional groups.

6 Environmental fate properties

The same comments about sources of data, reliability scoring and use of supplemental information apply as for Section 5.

6.1 Degradation

6.1.1 Abiotic degradation

6.1.1.1 Hydrolysis

The EU REACH registration dossier contains a data waiver for hydrolysis. The justification given is that PFBE is a highly volatile liquid of low water solubility (15.6 mg/L). Volatilisation from the aquatic environment is expected to be rapid, based on the estimated Henry's Law constant (3 - 100 atm.m^3/mol) and a high vapour pressure (22 kPa at 20 °C). Consequently, detectable concentrations will be hard to achieve in the aquatic environment.

The Environment Agency considers that the substance does not contain readily hydrolysable functional groups, so agrees hydrolysis is unlikely to be a major degradation pathway.

6.1.1.2 Phototransformation in air

No relevant information is available in the EU REACH registration dossier. A statement in the PBT assessment section of the dossier indicates that PFBE is expected to have a short atmospheric lifetime of 6.4 hours, although no supporting information is provided (ECHA, 2022a).

Direct photolysis of a carbon-fluorine chain is expected to be very slow, with stability expected to be sustained for more than 1,000 years (Environment Canada, 2012). Slow indirect photodegradation in air has been suggested for perfluorooctanoic acid (PFOA) by analogy with shorter chain perfluorinated acids, with an atmospheric lifetime of 130 days.

The Environment Agency considers that PFBE, like highly fluorinated chemicals, is likely to have a long atmospheric half-life, although the double bond at the end of the alkyl chain may be susceptible to hydroxyl radical attack. AOP v1.91 (EPISuite^{TM} v4.11) indicates an atmospheric half life of 6.42 hours based on indirect photolysis of the double bond. Gomis *et al*. (2015) note that the predictive power of AOPWIN for PFAS is limited despite the inclusion of some fluorinated substances in the training set, and that based on comparisons of predicted and measured photodegradation rates for 7 fluorinated substances they expect that AOPWIN may underestimate the true half-life in air.

6.1.1.3 Phototransformation in water

No studies are available from the EU REACH registration dossier or from published data sources.

6.1.1.4 Phototransformation in soil

No studies on are available from the EU REACH registration dossier or from published data sources.

6.1.2 Biodegradation in water

6.1.2.1 Measured data

Table 6.1 Summary of screening biodegradation studies

Method	Results	Reliability	Reference
OECD TG 301 D (Ready Biodegradability: Closed Bottle Test) GLP	Not readily biodegradable 15.9% degradation after 28 days (DOC removal)	Registrant: 1 (key study)	Unnamed study report (2001), cited in ECHA, 2022a

The EU REACH registration dossier summarises a biodegradation screening study (OECD, 1992; OECD TG 301 D; Ready Biodegradability: Closed Bottle Test) carried out according to GLP to determine the biodegradability of PFBE in water (Unnamed Study report, 2001; ECHA 2022a). PFBE was solubilised in 1,4-dioxane, and biodegradation investigated over a 28-day period in closed bottles using microorganisms from a sewage treatment plant mainly fed with municipal wastewater. PFBE was biodegraded by 15.9 % over 28 days. The substance is volatile but use of closed bottles should have minimised the likelihood of significant losses through evaporation.

PFBE is therefore not readily biodegradable. No toxic effects on the microorganisms were observed and the reference substance (sodium benzoate) was degraded by 78.4 % during the same timeframe.

The Environment Agency notes that 1,4-dioxane is not a standard solvent for ready biodegradability testing. The result appears to be acceptable although there is insufficient detail in the summary to confirm that the validity criteria were met.

6.1.2.2 Predicted data

The Environment Agency consulted the US EPA CompTox (US EPA, 2022a) database as well as EPIsuite^{TM} v4.11 for estimated water biodegradation.

- The predicted biodegradation half-life from CompTox is 4.46 days. The QSAR Model Reporting Format (QMRF) states that the endpoint units are log days. The antilog (assuming base e) equals 86.5 days. However, PFBE falls outside the applicability domain of the model, so this prediction is considered unreliable.
- Predicted half-life in water based on BIOWIN is 4 320 hours (EPIsuite^{TM} v4.11), The validation set contained several PFCs (see Appendix C) and it is likely that the predicted value for PFBE falls within the applicability domain of the model. Nevertheless, Gomis *et al*. (2015) note that the predictive power of BIOWIN3 for PFAS is limited. This prediction should therefore be treated with caution

6.1.2.3 Data from structural analogues

Not considered.

6.1.2.4 Discussion

The only experimental study available indicates that PFBE is not readily biodegradable. Although some details are missing from the robust study summary, the Environment Agency does not consider that further information is required.

The reported degree of mineralisation (up to 15.9 % over 28 days) is unexpected for such a highly fluorinated substance. The transformation products were not identified but could be shorter perfluorinated chains following removal of the ethene group, either perfluoropentanoic acid or perfluorobutanoic acid. These would be expected to be highly resistant to further transformation.

6.1.3 Biodegradation in sediment

This is a standard information requirement for the level of EU supply, but a data waiver is presented in the EU registration dossier, stating that neither direct nor indirect aquatic nor sediment exposure is likely due to high volatility.

No further information is available from published data sources.

6.1.4 Biodegradation in soil

A data waiver is presented in the EU registration dossier for this endpoint, stating that neither direct nor indirect soil exposure is likely due to high volatility.

No further information is available from published data sources.

6.1.5 Summary and discussion on degradation

The EU registration dossier provide waivers for hydrolysis and simulation degradation studies. The justification for these waivers state that PFBE is too volatile and/or of too low water solubility.

The Environment Agency considers that hydrolysis is unlikely to be a significant degradation mechanism due to the chemical structure. Slow phototransformation in air is a possibility.

The substance is not readily biodegradable, though may be a source of perfluoropentanoic acid or perfluorobutanoic acid in the environment. There are no environmental simulation data so a half-life in relevant media is not available.

6.2 Environmental distribution

6.2.1 Adsorption/desorption

6.2.1.1 Measured data

The EU REACH registration includes an organic carbon-water partition coefficient (K_{OC}) study performed according to OECD TG 121 (HPLC method) (OECD, 2001) in accordance with GLP (Unnamed study report, 2001). The EU registration dossier assigned a Klimisch score of 1 (reliable without restriction).

Eight reference substances were used (formamide, acetanilide, atrazine, monuron, tiapenthenol, linurone, fenthione, and trigluraline, with calculated log K_{OC} values ranging from 1.61 to 3.94). The log K_{OC} of PFBE was 2.96, based on a retention time of 8.08 minutes which was within the range covered by the reference substances.

The calculated log K_{OC} of PFBE is moderately high and suggests that despite high volatility this substance may adsorb to soils or sediments (contrary to the claims made in the EU registration dossier that direct or indirect exposure of these compartments is unlikely). The Environment Agency notes that the HPLC method may overcome the handling issues associated with volatile substances that would occur if an alternative study design were used to determine this endpoint (i.e. the OECD TG 106 batch equilibrium method (OECD, 2000)). However, OECD TG 121 is an indirect method which uses the stationary phase of the column as a surrogate for organic matter in the environment. It provides an estimate of K_{OC} only.

6.2.1.2 Predicted data

For comparative purposes, the Environment Agency has considered readily available QSAR software to test how they perform for this type of substance. The US EPA CompTox dashboard contains a predicted K_{OC} of 452 L/kg (log K_{OC} of 2.67) (US EPA, 2022a).

- The Environment Agency used KOCWIN v2 model prediction within EPISuite™ v4.11 to estimate a log K_{OC} of 3.9. The validation set contained several PFCs (see Appendix C) and it is likely that the predicted value for PFBE falls within the applicability domain of the model.

6.2.1.3 Data from structural analogues

Experimentally derived log K_{OC} values were available for two of the three selected structural analogues of PFBE:

- 3,3,4,4,5,5,6,6,7,7,8,8-dodecafluorodeca-1,9-diene: log K_{OC} 4.3 (ECHA, 2022c; HPLC estimation method OECD TG 121)
- 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooct-1-ene: log K_{OC} 2.65 (ECHA, 2022d; HPLC estimation method OECD TG 121)

Since the first substance has two non-fluorinated double bonds, it is likely to be more adsorptive than PFBE so is probably less relevant.

6.2.1.4 Recommended value

An indirectly measured log K_{OC} of 2.96 is considered reliable without restriction in the EU registration dossier. This is broadly consistent with predicted values (2.67 and 3.9), and similar to the log K_{OC} 2.65 of the larger analogue 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooct-1-ene.

The Environment Agency considers that the available data indicates a log K_{OC} around 3, and therefore the value presented in the EU registration dossier of **2.96** is appropriate for further evaluation.

6.2.2 Volatilisation

6.2.2.1 Measured data

No measured data were available in the literature.

6.2.2.2 Calculated data

The EU REACH registration dossier includes a Henry's Law constant (HLC) calculation using the following equation:

$$\text{HLC} = \frac{\text{1 standard atmospheric pressure (Pascals)} \times \text{molecular weight}}{\text{water solubility (mg/L)}}$$

This is 101 300 Pa × (246/15.6 mg/L (Section 5.3.1)) = 1 597 423 Pa m^3/mol or 15.77 atm m^3/mol. The Environment Agency notes that this result is wrong, as it ignores the vapour pressure of PFBE (Section 5.1.1) and litres must be converted to m^3.

The Environment Agency recalculated the HLC using the equation from the ECHA R7.a guidance text (ECHA, 2017) using the following variables. The water solubility of 15.6 mg/L converts to 6.34×10^{-5} mol/L and 6.34×10^{-2} mol/m^3, using the molar weight of PFBE as 246 g. The vapour pressure is 22 kPa or 0.2171 atm at 20 °C (Section 5.1.1). Ideally, the Environment Agency would adjust the vapour pressure to 25 °C using the Clausius-Clayperon equation. This is not possible as the enthalpy of vaporisation of PFBE is unknown.

$$\text{HLC} = \text{vapour pressure (Pa)} / \text{water solubility (mol/m}^3\text{)}$$

$$= 347\ 000\ \text{Pa.m}^3\text{/mol or } 3.42\ \text{atm.m}^3\text{/mol}$$

There is some uncertainty in the input parameters, which affects the reliability of this estimate.

6.2.2.3 Predicted data

The US EPA CompTox dashboard contained a predicted HLC value for PFBE (US EPA, 2022a). For comparative purposes, the Environment Agency generated a HLC constant through EPISuite^{TM} v4.11. These values are presented in Table 6.2. The Environment Agency has converted the values from atm.m^3/mol to Pa.m^3/mol.

Table 6.2 Predicted Henry's Law constant for PFBE

Source	HLC
EPISuite™ Estimation programme **HENRYWIN v3.1**	1.125×10^7 Pa.m^3/mol or 111 atm.m^3/mol (Environment Agency) 440.763 Pa.m^3/mol or 0.00435 atm.m^3/mol (CompTox)
CompTox US EPA, 2022a (OPERA)	440.763 Pa.m^3/mol or 0.00435 atm.m^3/mol

In silico predicted values should always be treated with caution where substances in the training set and external test set are not visible. The training and validation sets for the HENRYWIN model contained several PFCs (see Appendix C) and it is likely that the predicted value for PFBE falls within the applicability domain of the model. However, the prediction relies on predicted values for vapour pressure and water solubility, so the output should be treated with additional caution. The CompTox prediction falls outside the applicability domain of the OPERA model and is therefore unreliable.

6.2.2.4 Data from structural analogues

A Henry's Law constant was only available for one of the structural analogues of PFBE: 263 952 Pa.m^3/mol for 3,3,4,4,5,5,6,6,7,7,8,8-dodecafluorodeca-1,9-diene calculated in the EU registration dossier; HLC=(VPxMOLW)/WS) (ECHA, 2022c).

6.2.2.5 Recommended value

The relatively high vapour pressure and moderate water solubility implies that PFBE will tend to partition to air from water under environmentally relevant conditions. There is uncertainty in the input parameters and QSARs, but in the absence of further information the Environment Agency recommends the calculated Henry's Law constant of **347 000 Pa.m^3/mol (3.42 atm.m^3/mol)** for modelling purposes (as it is derived using measured water solubility and vapour pressure values).

6.2.3 Distribution modelling

To estimate the distribution of PFBE in the environment, the Environment Agency has run the EQC v3.0 Mackay Level III fugacity model using the input parameters indicated in Table 6.3.

Table 6.3 Estimated distribution of PFBE

Input Parameter	Value	
Molecular mass	246.07 g/mol	
Melting point	<-20 °C	
Water solubility	15.6 mg/L	
Vapour pressure	22 000 Pa	
Henry's Law constant	347 000 Pa m^3/mol	
Log KOW	4.13	
Half-life in air (hours)[a]	2.1 x 10^{41}	
Half-life in water (hours)[a]	2.1 x 10^{41}	
Half-life in soil (hours)[a]	2.1 x 10^{41}	
Half-life in sediment (hours)[a]	2.1 x 10^{41}	
Model output	Scenario 1 - all emissions to water	Scenario 2 - all emissions to air
Air %	20.0	100.0
Water %	79.9	0.0
Soil %	0.2	0.0

Input Parameter	Value	
Sediment %	0.0	0.0

Note: a - The upper bound value for biodegradation of a non-readily biodegradable substance in EUSES is 1 x 10^{40} days to represent infinity (equivalent to 2.1 x 10^{41} hours).

Based on these input parameters and the assumption that PFBE does not degrade in the environment, the model predicts that nearly all the substance would remain in the water compartment if released to water. If released to air, all the substance would remain in the air compartment. The reliability of this modelling is uncertain because of the assumptions around half-life in different compartments.

6.2.4 Long-range transport potential

The OECD has produced a decision support tool for estimating the long-range transport potential (LRTP) of organic chemicals at a screening level (Wegmann *et al*., 2009). It is a steady state non-equilibrium model in a standardised evaluative environment, predicting three characteristics that can be used to indicate the LRTP of a substance: Characteristic Travel Distance (CTD), Transfer Efficiency (TE) and overall persistence (P_{OV}).

To estimate the LRTP of PFBE, the Environment Agency has performed calculations using the input parameters indicated in Table 6.4.

Table 6.4 Estimated long-range transport potential of PFBE

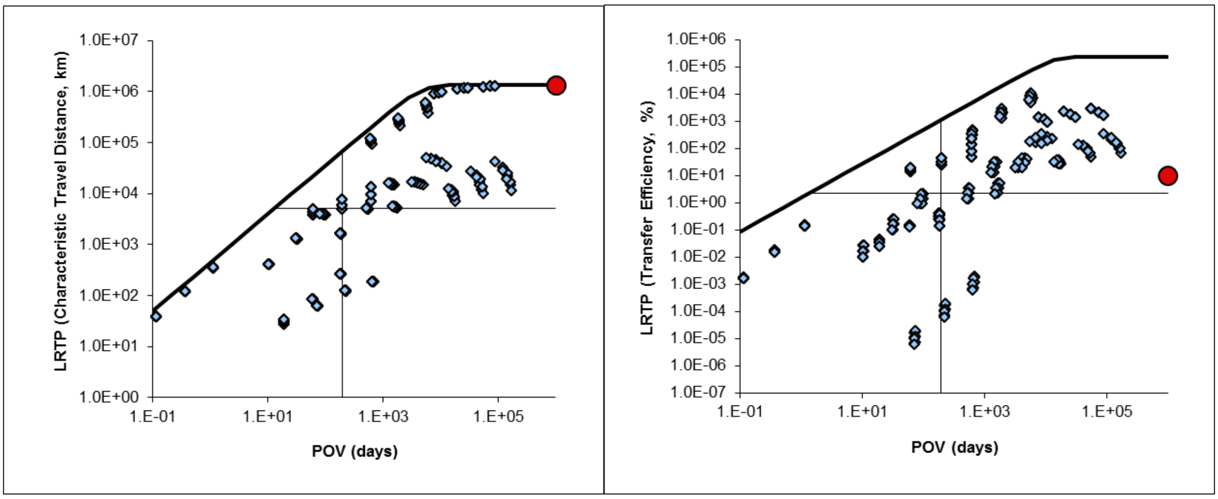
Input Parameter	Value
Molecular mass (g/mol)	246.07
Log K_{AW} [a]	2.17
Log K_{OW}	4.13
Half-life in air (hours)[b]	2.1 x 10^{41}
Half-life in water (hours)[b]	2.1 x 10^{41}
Half-life in soil (hours)[b]	2.1 x 10^{41}
LRTP output parameter	
Characteristic Travel Distance (km)	1 350 000
Transfer Efficiency (%)	1 055
P_{OV} (days)	1.26 x 10^{40}

Note: a - This is the log of the dimensionless HLC calculated using Equation R.16-5 of ECHA (2016).

b -The upper bound value for biodegradation of a non-readily biodegradable substance in EUSES is 1 x 10^{40} days to represent infinity (equivalent to 2.1 x 10^{41} hours).

The OECD LRTP screening tool allows comparisons of the CTD and TE characteristics for a range of substances, some of which are POPs, provided in Figure 6.1.

Figure 6.1 Long-range transport potential of PFBE for predictive modelling



Note: In the left hand graph the x axis is overall persistence in days (Pov) and the y axis is the Characteristic Travel Distance (km). In the right hand graph the x axis is overall persistence in days (Pov) and the y axis is the Transfer Efficiency (%).

Based on this screening tool and the assumption that PFBE does not degrade in the environment, it appears that PFBE may be capable of long-range transport as it falls into the top right quadrant of Figure 6.1. The reliability of this modelling is uncertain because of the assumptions around half-life in different compartments, particularly air. Evidence of occurrence (or not) of PFBE in the Arctic and other remote regions also needs to be taken into account (noting the proximity of industrial activity and population centres). This is beyond the scope of this evaluation.

6.3 Bioaccumulation

6.3.1 Bioaccumulation in aquatic organisms

6.3.1.1 Measured data

A data waiver is presented in the EU registration dossier for this endpoint, on the basis that neither direct nor indirect aquatic or sediment exposure is likely due to high volatility.

No further information is available from published data sources.

6.3.1.2 Predicted data

A fish bioconcentration factor (BCF) can be calculated based on log K_{OW} and the QSAR equation in ECHA (2017c). The Environment Agency has used the experimental log K_{OW} of 4.13 to calculate a BCF of 646. The reliability of this QSAR for this type of substance is unknown.

The Environment Agency also used EPISuite™ v4.11 software to predict the BCF of PFBE using the values in Section 5 of this report. A predicted BCF of 247 L/kg wet weight (ww) was generated using BCFBAF v3.01. The validation set contained several PFCs (see Appendix C) and it is likely that the predicted value for PFBE falls within the applicability domain of the model. The Henry's Law Constant (HLC) cannot be overridden in EPISuite™. The BCF prediction therefore relies on the predicted HLC of the model which differs from the calculated HLC. The BCF prediction should therefore be treated with caution.

The US EPA CompTox dashboard contains predicted fish BCF values for PFBE generated from both the OPERA and T.E.S.T. software (US EPA, 2022a). The OPERA model predicts a BCF of 92, but notes that PFBE is outside of the applicability domain, so the prediction is not valid. The T.E.S.T. model predicts a BCF of 234, and structural analogues of PFBE are included in the training set so this value might be more reliable.

The PubChem database (NCBI, 2022) contains a predicted BCF of 370 for PFBE, and the RSC ChemSpider portal includes two BCF values: 1 393 generated from the BCFWIN v2.17 software and 387 from ACD/Labs (RSC, 2022). None of these sources provide further information.

6.3.1.3 Data from structural analogues

One experimental study is available for 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooct-1-ene (ECHA, 2022d). The study was performed over 60 days according to OECD TG 305 (1996) and GLP with Common Carp *Cyprinus carpio* via the aqueous phase at a nominal test concentration of 0.1 and 1.0 µg/L. Due to the substance's volatility, the study used special test vessels and a flow-through test design with a high daily renewal rate, which resulted in measured concentrations close to nominal. The steady-state BCF was 380 (1 µg/L) or 300 (0.1 µg/L) based on whole body wet weight.

6.3.1.4 Recommended value

There are no measured data for the substance itself. Predicted BCF values of variable reliability range from 234 to 646 (with 1 393 as an outlier, the reliability of which cannot be evaluated). These compare well with a measured BCF of 300 to 380 for a higher molecular weight analogue.

In the absence of experimental data for the substance itself, the Environment Agency recommends a predicted BCF of **646** as a reasonable worst case for the purposes of this evaluation.

6.3.2 Terrestrial bioaccumulation

The EU registration dossier does not assess the potential for terrestrial bioaccumulation.

No information on bioaccumulation is available from the available mammalian toxicity studies. Evidence from other highly fluorinated substances suggests that terrestrial bioaccumulation (or bioaccumulation in air-breathing organisms) may be more relevant for some PFAS than aquatic bioaccumulation, although this is mainly related to the ability of perfluorocarboxylic acids to bind to proteins.

In terms of bioaccumulation in air-breathing organisms, the screening criteria are log $K_{OW} > 2$ and log $K_{OA} > 5$ (ECHA, 2017c). Although the log K_{OW} 4.13 exceeds the first threshold the log K_{OA} of 1 (Section 5.5.4) does not, so this criterion is not met.

6.3.3 Summary and discussion of bioaccumulation

The log K_{OW} of 4.13 suggests that PFBE has potential for bioaccumulation by partitioning to lipids. However, it appears unlikely to bioaccumulate significantly in aquatic gill-breathing organisms, based on a predicted fish BCF of 646. The value is comparable to similar low BCFs seen for other PFAS.

The bioaccumulation potential of PFBE in air-breathing organisms is uncertain but there are no indications of concern based on currently available data.

7 Ecotoxicology

7.1 Aquatic compartment

The same comments about sources of data, reliability scoring and use of supplemental information apply as for Section 5. The Environment Agency notes that PFBE has a low solubility in water (Section 5.3) and high Henry's Law constant (Section 6.2.2) which indicates that the substance will tend to volatilise from water to air. Measurement of test concentrations is therefore important for aquatic toxicity studies, as consistent exposure concentrations may be difficult to maintain (especially in static test systems).

7.1.1 Fish

7.1.1.1 Short-term (acute) toxicity

Table 7.1 Summary of acute toxicity to fish

Method	Species	Analytical method	Results	Reliability	Reference
Ecotoxicological testing of petroleum products (CONCAWE 1992) and aquatic toxicity testing of lubricants by ASTM (standard protocol 06081-97) Similar or equivalent to OECD TG 203 (semi-static) GLP	Zebra fish (*Danio rerio*)	Confidential	96-h LC_{50} >1.86 mg/L based on the arithmetic mean initial measured concentration	Registrant: 1 (key study)	Unnamed (2001) cited in ECHA, (2022a)

One acute fish toxicity study was presented in the EU REACH registration dossier as the key study (Unnamed, 2001, cited in ECHA, 2022a). The CONCAWE and ASTM methods were reported to be similar to OECD TG 203 (OECD, 2019), and the study was carried out in accordance with GLP. The test was conducted using PFBE with an analytical purity of 96%. Semi-static conditions were used with a 24-hour renewal period, and volatile loss of PFBE from the test system was minimised through the use of closed test vessels. The test temperature was maintained at 22±1 °C.

Test solutions were prepared as WAFs, with initial nominal loading rates of 0 (control), 100, and 1 000 mg/L. Details about how the WAF was prepared are provided on the ECHA website. The first portion of the WAF was used to rinse the test vessels to saturate the surfaces. After filling, the test vessels were sealed immediately and only opened again to introduce the test organisms and "*again at the end of the test*" (*sic* – presumably between renewals too). Care was taken to ensure that any undissolved material was not transferred to the test vessels. The WAFs were not stored for more than 1 to 2 hours prior to testing. The concentration of PFBE in the WAFs was measured in vessels without fish at 0 h, 24 h (end of initial exposure), 24 h (fresh solutions), 48 h (fresh solutions), 72 h (fresh solutions), and 96 h (end of exposure). Prior to chemical analysis, 100 mL aliquots of test media were filtered to remove particulate matter. The sieve was pre-rinsed with the corresponding WAF prior to filtration. Concentrations of PFBE ranged from 0.11 to 0.75 mg/L (mean 0.34 ± 0.29 mg/L) and 1.56 to 2.57 mg/L (mean 1.86 ± 0.35 mg/L) for loading rates of 100 and 1 000 mg/L, respectively. During the initial exposure period of 24 h the concentration of PFBE decreased 19 to 27 % and 34 to 44 % for the loading rates of 100 and 1 000 mg/L, respectively.

All measurements indicated that PFBE was below the water solubility of 15.6 mg/L (see Section 6.3.4). The measured concentrations were used in the EU registration dossier to generate the concentration-effect relationship. The pH ranged from 7.48 to 8.23 and mean dissolved oxygen was greater than 79% saturation for all vessels.

No significant mortality was observed in either treatment or control groups (10% in mid and high group, but within tolerable limits of study). The validity criteria of < 10% mortality in control groups and > 60% dissolved oxygen (DO) saturation were met. Most other test parameters were closely related to the standards recommended in OECD TG 203 (OECD, 2019). Information on the frequency of feeding before the test and the intervals for the measurement of pH and temperature were not available in the registration dossier.

The results were reported as 96-h NOEC ≥ 1 000 mg/L and EC_{50} > 1 000 mg/L (nominal WAFs), corresponding to 96-h NOEC ≥ 1.86 mg/L and EC_{50} > 1.86 mg/L based on the measured concentrations. The EU registration dossier consider the study to be reliable without restriction (Klimisch score 1).

The Environment Agency notes that the measured concentrations were an order of magnitude lower than the measured water solubility (15.6 mg/L). It is not clear why this should be the case, because steps were taken to minimise evaporative losses during the test. In addition, WAFs are usually prepared for complex mixtures whose constituents have a variety of different solubilities (like petroleum products). PFBE is a mono-constituent substance of moderate water solubility, so it is possible that a different test solution preparation technique (or flow-through conditions) might have achieved greater dissolved concentrations.

7.1.1.2 Long-term (chronic toxicity)

Long-term fish toxicity tests are not available, and the EU registration dossier uses a data waiver (no details of this waiver are provided on the ECHA website).

7.1.2 Aquatic invertebrates

7.1.2.1 Short-term (acute) toxicity

Table 7.2 Summary of acute toxicity to aquatic invertebrates

Method	Species	Analytical method	Results	Reliability	Reference
Ecotoxicological testing of petroleum products (CONCAWE 1992) and aquatic toxicity testing of lubricants by ASTM (standard protocol 06081-97) Similar or equivalent to OECD TG 202 (static) GLP	*Daphnia magna*	Confidential	Acute immobilisation test 48-h EC_{50} >1 mg/L	Registrant: 1 (key study)	Unnamed study report (2001) cited in ECHA (2022a)

One acute aquatic invertebrate toxicity study is included in the EU REACH registration dossier as the key study (Unnamed 2001, cited in ECHA 2022a). This study was reported to be similar or equivalent to an OECD TG 202 (OECD, 2004) study and carried out to GLP using *Daphnia magna*. Substance purity and test solution preparation was identical to the acute fish test, with WAF loading rates of 0, 100 and 1 000 mg/L. Static exposure conditions were used.

The validity criteria for <10% immobility in the controls and ≥3 mg/L DO were met. The pH ranged from 8.64 to 8.99 and the test temperature was maintained at 20±1 °C.

Measured concentrations were 0, 0.27, and 1.0 mg/L, respectively, on day 0; and 0, 0.19, and 0.80 mg/L, respectively, on day 2. Losses were reportedly due to high volatility.

No significant increase in immobility was seen for any of the treatment groups compared to controls. The 48-h NOEC was reported as ≥ 1 mg/L, with a 48-h EC_{50} ≥ 1mg/L. The EU registration dossier consider the study to be reliable without restriction (Klimisch score 1).

The Environment Agency notes that the measured concentrations were around 1 to 2 orders of magnitude lower than the measured water solubility (15.6 mg/L). Losses of around 20 to 30 % were observed between day 1 and day 2, which the EU registration dossier attributes to evaporation even though steps were taken to minimise this. WAFs are usually prepared for complex mixtures whose constituents have a variety of different solubilities (like petroleum products). PFBE is a mono-constituent substance of moderate water solubility, so it is possible that a different test solution preparation technique might have achieved greater dissolved concentrations. As a minor point, the Environment Agency considers that the result should be reported as a 48-h EC_{50} ≥ 0.8 mg/L, as this was the highest concentration measured in the test.

7.1.2.2 Long-term (chronic) toxicity

Long-term invertebrate toxicity tests are not available, and the EU registration dossier uses a data waiver (no details of this waiver are provided on the ECHA website).

7.1.3 Algae and aquatic plants

Table 7.3 Summary of toxicity to algae

Method	Species	Analytical method	Results	Reliability	Reference
Ecotoxicological testing of petroleum products (CONCAWE 1992) and aquatic toxicity testing of lubricants by ASTM (standard protocol 06081-97) Similar or equivalent to OECD TG 201 (static) GLP	*Pseudo-kirchneriella subscapita*	Confidential	Algal growth rate 72-h E_rC_{50} >1.5 mg/L 72-h NOE_rC ≥1.5 mg/L	Registrant: 1 (key study)	Unnamed study report (2001), ECHA (2022a).

The algal growth inhibition study presented in the EU REACH registration dossier as the key study (Unnamed study report, 2001, cited in ECHA 2022a). The methods were reported to be similar or equivalent to OECD TG 201 (OECD, 2011) and the study was carried out in accordance with GLP using the green alga *Pseudokirchneriella subscapita*. Substance purity and test solution preparation was identical to the acute fish test, with WAF loading rates of 0, 100 and 1 000 mg/L. Static exposure conditions were used. The starting cell concentration was 1 000 cells/mL and the test vessels were completely full and sealed. The purpose of the decreased cell number (10 times lower than recommended in the guideline) was to prevent the development of a large biomass by the end of the study. This was considered necessary because of the risk of depleting the carbonate concentration which could have made the solutions alkaline and artificially limited the growth rate.

The cell concentrations were determined at the start of the test and after 24, 48 and 72 h. The volume of test solution removed for evaluation and that displaced by the stopper were replaced using spare WAF which had been stored in a sealed vessel. A separate spare vessel was prepared for each replacement interval (1 vessel per test concentration). The reason was to prevent re-equilibration of the volatile test substance from the WAF to the head-space above the WAF. The culture vessels were incubated at 22 ± 1 °C.

Measured concentrations were <0.05, 0.92, and 1.52 mg/L for the 3 loading rates, respectively, at the start of the test. The concentration of PFBE was below the detection limit of 0.05 mg/L in all vessels but one at the end of the test (the single positive detection was a concentration of 0.11 mg/L in one of the 5 vessels used at the 1 000 mg/L loading rate). Test vessels had to be opened daily for sampling, so the EU registration dossier attributes the decline of PFBE concentration to evaporation during the sampling procedure.

No significant inhibitory effect on growth rate was observed compared to the controls (an increase in biomass (36.5% compared to control) was observed at the highest loading rate by the end of the test). The 72-h NOE_rC was reported as ≥1.5 mg/L with the 72-h E_rC_{50} >1.5 mg/L. The EU registration dossier considers the study to be reliable without restriction (Klimisch score 1).

The Environment Agency notes that the initial measured concentrations were an order of magnitude lower than the measured water solubility (15.6 mg/L). Almost a complete loss of test substance had occurred by 72 h, which is presumably due to evaporation, but may possibly also be due to adsorption to the algal cells. WAFs are usually prepared for complex mixtures whose constituents have a variety of different solubilities (like petroleum products). PFBE is a mono-constituent substance of moderate water solubility, so it is possible that a different test solution preparation technique might have achieved greater dissolved concentrations. Given the observed drop in concentration, it is unclear how long the cells were exposed to significant amounts of PFBE, and so it may be more precautionary to report the results as a 72-h E_rC_{50} >0.05 mg/L, and a 72-h NOE_rC ≥0.05 mg/L.

7.1.4 Sediment organisms

No relevant information is available in the EU REACH registration dossier. The EU registration dossier includes a data waiver, arguing that the substance has only moderate affinity to sediment (log K_{OC} 2.96), has high volatility from water, and direct and indirect exposure of sediment is unlikely (ECHA 2022a).

7.1.5 Other aquatic organisms

No other relevant information is available.

7.2 Terrestrial compartment

No relevant information is available in the EU REACH registration dossier. The EU registration dossier includes a data waiver, arguing that the substance has only moderate affinity to soil (log K_{OC} 2.96), has high volatility, and direct and indirect exposure of soil is unlikely (ECHA 2022a).

7.3 Microbiological activity in sewage treatment systems

A test to determine the toxicity of PFBE to sewage microorganisms is not available and the EU registration dossier uses a data waiver (no details of this waiver are provided on the ECHA website). The Environment Agency notes that no toxicity to the inoculum was observed in the ready biodegradation test (see Section 6.1.2).

7.4 Atmospheric effects

The Henry's Law constant indicates that PFBE is likely to significantly partition to air (see Section 6.2.2). No data about biotic effects (e.g. to plants) from aerial exposure are available in the EU REACH registration dossier (ECHA, 2022a), but this is not a standard information requirement.

The available data in the EU REACH registration dossier suggest that PFBE is unreactive to ozone, and therefore is unlikely to be an ozone depleting substance.

PFCs are known to be potent greenhouse gases, and this is considered further in Section 9.5.

8 Mammalian toxicology

The following information is taken directly from the ECHA public dissemination website entry for PFBE (ECHA, 2022a). The focus is on those mammalian endpoints which are potentially relevant for determination of the substance as Toxic ('T') according to the REACH Annex 13 criteria (see Section 9.3) or for a wildlife secondary poisoning assessment (see Section 9.5). No human health hazard assessment has been undertaken. The study details and their reliability (Klimisch) scores are as presented in the EU registration dossier and the Environment Agency has not evaluated this information.

8.1 Toxicokinetics

No information on toxicokinetics have been presented in the EU registration dossier.

8.2 Repeated dose toxicity

Table 8.2 Summary of mammalian repeated dose toxicity endpoints

Method	Species	Brief study details	Results	Reliability (Klimisch) score	Reference
Short-term repeated dose toxicity: inhalation OECD TG 412 (Subacute inhalation toxicity: 28-day study) GLP	Rat (Wistar)	Nose only exposure, analytical verification of doses / concentrations using Flame ionisation detector (FID) 28-day exposure 6 hours per day 401, 2069, and 9879ppm doses N=5/sex/dose	10 000 ppm haematological effect in males Clinical biochemistry effects in males at 2 000 ppm and females at 10 000 ppm Histopathological effects seen – non-neoplastic NOAEC 2 000 ppm (2 069±179 ppm measured), despite effects seen at 2 000 ppm	Registrant: 1 (key study)	Unnamed study report (2001) cited in ECHA (2022a)

Method	Species	Brief study details	Results	Reliability (Klimisch) score	Reference
Sub-chronic toxicity: inhalation OECD TG 413: Sub-chronic inhalation toxicity: 90 Day study GLP	Rat (Wistar)	PFBE >99.9% purity Nose only exposure N=10 male and 10 female per group 0, 1 000, 3 000 and 10 000 ppm with analytical verification of dose 6 hours per day for 5 days per week for 90 days	In males decreased mean body weight gain at all exposure levels (0.9, 0.86, and 0.89 times control respectively) Haematological (immunological) effect at 3 000 and 10 000 ppm NOAEL 10 000 ppm (despite effects seen)	Registrant: 1 (key study)	Unnamed study report (2017) cited in ECHA (2022a)

Method	Species	Brief study details	Results	Reliability (Klimisch) score	Reference
Short-term repeated dose toxicity: inhalation Similar to OECD TG 412: Subacute inhalation toxicity 28-day study	CD1 rats	PFBE 99% purity Whole body inhalation study N=10 male and 10 female per dose (analytical confirmation of dose) Males: 0, 541, 4 750, and 46 300 ppm Females: 0, 473, 5 140 and 46 800 ppm 6 hours per day for 5 days per week for 28 days	Haematological effects observed at 50 000 ppm in males and 5 000 and 50 000 ppm in females Increased liver and kidney weight relative to body weight in males at 50 000 ppm, increased kidney weight only in females at same dose. NOAEC for clinical chemistry 500 ppm NOAEC for histopathology 50 000 ppm	Registrant: 1 (supporting study)	Unnamed study report (1981) cited in ECHA (2022a)

8.3 Mutagenicity

Three *in-vitro* genetic toxicity studies are included in the EU REACH registration dossier, these are briefly summarised in Table 8.3.

Table 8.3 Summary of mammalian mutagenicity endpoints

Method	Species	Brief study details	Results	Reliability (Klimisch) score	Reference
In vitro gene mutation study in bacteria Bacterial Reverse Mutation Assay, OECD TG 471 GLP	*Salmonella typhimurium* and *Escherichia coli* strains	PFBE 100% purity With and without metabolic activation (S9 rat liver homogenate) 0, 0.062, 0.158, 0.556, 1.667, and 5.0 µL/plate	Negative (no adverse effects reported at these concentrations) The test article is not mutagenic with or without metabolic activation under the test conditions Negative control slightly elevated revertants	Registrant: 1 (key study)	Unnamed study report (2010) cited in ECHA (2022a)
In vitro cytogenicity/ chromosome aberration study in mammalian cells Mammalian Chromosome Aberration Test, OECD TG 473 GLP	Chinese hamster Ovary (CHO)	PFBE 100% purity With and without metabolic activation (S9 liver homogenate) Test 1: 0, 600, 1 230 and 2 460 µg/mL Test 2: 0, 100, 1 250 and 2 460 µg/mL	Negative for genotoxicity Cytotoxicity observed at 1 250 and 2 460µg/mL (in Executive summary the Registrants claim non-cytotoxic)	Registrant: 1 (key study)	Unnamed study report (2010) cited in ECHA (2022a)
In vitro gene mutation study in	Mouse lymphoma L5178Y cells	PFBE 100% purity. With and without	Negative, not mutagenic/ genotoxic to TK locus of L5178Y	Registrant: 1 (key study)	Unnamed study report (2010) cited in

Method	Species	Brief study details	Results	Reliability (Klimisch) score	Reference
mammalian cells Mammalian Cell Gene Mutation Test, OECD TG 476 GLP		metabolic activation (S9 liver homogenate with cofactors) 0, 1.2, 2.4, 4.9, 7.0, and 10 mmol/L doses	mouse lymphoma cells Slight cytotoxicity noted in the presence of S9		ECHA (2022a))
In vitro gene mutation study in bacteria Similar to guideline study	*Salmonella typhimurium*	PFBE 99% purity With and without metabolic activation (S9 rat liver homogenate) 0, 100, 500, 1 000, 5 000 and 10 000 µg/plate	Negative (no adverse effects at these concentrations). No supporting information	Registrant: 2 (supporting study)	Unnamed study report (1980) cited in ECHA (2022a)

8.4 Carcinogenicity

No information is available in the EU REACH registration dossier.

8.5 Toxicity to reproduction (effects on fertility and developmental toxicity)

Table 8.4 Summary of mammalian reproductive toxicity endpoints

Method	Species	Brief study details	Results	Reliability (Klimisch) score	Reference
Developmental Toxicity test. Similar or equivalent to OECD TG 414 Prenatal developmental toxicity study.	Rat: CD	Inhalation (whole body) N=7 per exposure Analytical verification of doses 0, 994, and 70 700 ppm Mated females exposed daily for 6 hours from day 6-15 of gestation Decreased mean maternal body weight gain in high exposure group	Decreased mean maternal body weight gain in high exposure group NOAEC >70 000 ppm for dams NOAEC >70 000 ppm for embryotoxicity NOAEC >70 000 ppm for teratogenicity	Registrant: 2 (key study)	Unnamed study report (1981) cited in ECHA (2022a)

One reproductive toxicity study is included in the EU REACH registration dossier as the key study (Unnamed study report, 1981, cited in ECHA, 2022a). This study was conducted in 1981 and reported to be similar to OECD TG 414. The test substance was administered through inhalation to groups of rats (n=7, CD strain) at 0, 994, 70 700 ppm. Pregnant females received daily doses for 6 hours/day between day 6 and 15 of gestation.

There were no treatment-related effects on male or female foetuses.

Mean body weight gain was decreased in the highest exposure maternal group.

8.6 Summary of mammalian toxicology

Based on the available mammalian toxicology data, the EU registration dossier concludes that no effects were demonstrated in studies conducted at maximally attainable vapour concentrations, limit doses, or other limits imposed by safety considerations.

9 Environmental hazard assessment

9.1 Classification and labelling

9.1.1 Harmonised classification

PFBE does not have a harmonised classification under the EU Classification, Labelling and Packaging (CLP) Regulation ((EC) No. 1272/2008), nor a mandatory classification under UK CLP.

9.1.2 Self-classification

The EU REACH registration dossier proposes that the substance is Not Classified, and no environmental hazards are identified on ECHA's CLP inventory (ECHA, 2022b).

9.1.3 Conclusions for classification and labelling

PFBE is not readily biodegradable and there is no evidence that it degrades significantly via abiotic mechanisms in aquatic media (see Section 6.1). It is therefore considered to be "not rapidly degradable" for the purposes of hazard classification.

No experimentally derived values for fish BCF are available. The log K_{OW} exceeds 4 (4.13), so PFBE meets the bioaccumulation criterion for the purposes of hazard classification. Despite the limited reliability of predicted BCFs for this substance, the Environment Agency's preferred BCF of 646 also meets the bioaccumulation criterion (>500 L/kg).

Acute ecotoxicity studies are available for fish, aquatic invertebrates and algae (see Section 7). None demonstrated any adverse effects up to the concentration limits achieved. However, the maximum concentrations achieved were at least an order of magnitude below the measured water solubility limit of 15.6 mg/L. In addition, test concentration maintenance was poor in the invertebrate and algal tests, with the latter experiencing almost complete loss of substance over a 72-h period, despite efforts to limit volatilisation. Nevertheless, based on the available evidence, **Aquatic Acute classification is not required.** This is consistent with the UK supplier's view.

No adverse chronic effects were observed in the algal toxicity test, resulting in a 72-h NOEC of ≥1.5 mg/L based on TWA, although as noted above, there was a significant loss in test concentration during this study. In the absence of further long-term toxicity information for fish and aquatic invertebrates, classification as **Aquatic Chronic 4** is warranted because the substance is poorly water soluble, not rapidly degradable and meets the bioaccumulation criterion. The Environment Agency recommends that the UK supplier updates their self-classification to reflect these findings.

The human health hazard classification has not been considered.

9.2 Assessment of endocrine disrupting (ED) properties

The ecotoxicity dataset does not include any studies that assess ED potential and no additional information was identified during the literature search (Appendix A).

9.3 PBT and vPvB assessment

Persistence: No environmental half-life data are available for comparison with the definitive criteria in REACH Annex 13. PFBE is not readily biodegradable and there is no evidence that it degrades significantly via abiotic mechanisms in aquatic media (see Section 6.1). The EU REACH registration dossier includes a statement that any PFBE released to the environment will partition to atmosphere and that it would have a short atmospheric lifetime estimated as 6.4 hours, but no further details are provided. This information is used to conclude that the substance is neither persistent (P) nor very persistent (vP). However, the Environment Agency considers that PFBE meets the screening criterion for being P or vP.

Bioaccumulation: PFBE has a reported log K_{OW} of 4.13 (Section 5.4) which does not meet the REACH screening criterion for bioaccumulation (B), as it is below 4.5. The predicted fish BCF of 646 similarly falls below the definitive B criterion in REACH Annex 13 (>2 000 L/kg).

In terms of bioaccumulation in air-breathing organisms, the log K_{OW} of 4.13 meets the screening criteria (>2), but the log K_{OA} of 1 does not (as it is below 5).

Toxicity: In terms of aquatic toxicity, a 72-h NOEC of ≥1.5 mg/L is available for algae, which does not meet the REACH Annex 13 criterion for toxicity (T) of <0.01 mg/L (see Section 7). There are no chronic aquatic toxicity data for fish or aquatic invertebrates, but no acute toxicity has been observed for these taxonomic groups. PFBE therefore does not meet the screening criterion for being potentially T based on toxicity to aquatic organisms.

PFBE does not meet the T criterion based on mammalian toxicity as indicated by the industry self-classifications for human health hazards (see Section 9.1).

No information is available on ED potential.

Overall conclusion: PFBE screens as potentially P/vP, but does not screen as potentially B or T. It is therefore of low concern for PBT and vPvB hazards.

9.4 Groundwater hazard

Draft persistence, mobility and toxicity (PMT) criteria have been developed by the German Federal Environment Agency as intrinsic hazard criteria to identify substances that are difficult to remove during normal wastewater treatment practices and may be a threat to remote aquatic environments and drinking water sources, including groundwater (Arp and Hale, 2019). The criteria for P and vP are consistent with those in REACH Annex 13, whereas the mobile criterion is unique to PMT assessments. The T criteria include those in REACH Annex 13, in addition to considerations for carcinogenicity, effects via lactation, long-term toxicity to the general human population and ED potential.

There is no legal basis for these criteria under the REACH Regulation, but for completeness, a brief evaluation is included here.

Persistence: PFBE meets the screening criterion for being potentially P or vP (see Section 9.3).

Mobility: The measured log K_{OC} value of 2.96 (see Section 7.2.1) meets the criterion of being mobile (M) (log K_{OC} ≤4) and vM (log K_{OC} ≤3).

Toxicity: PFBE does not meet the T criterion based on aquatic or mammalian toxicity (see Section 9.1). No information is available on ED potential.

Overall conclusion: PFBE screens as potentially P/vP and M/vM, but not as T. It therefore meets the vPvM screening criteria. PFBE is a volatile liquid, and the influence of volatility is not considered under the criteria.

In addition, PFBE has the potential to degrade to perfluoropentanoic acid and perfluorobutanoic acid. An assessment of their properties (and other contributing substances) is outside scope of this evaluation. However, they are both likely to be vPvM, and so PFBE would be relevant in terms of any risk management associated with these “arrowhead” sunstances.

9.5 Greenhouse gas hazard

PFBE is a volatile liquid, and a significant proportion of emissions are expected to end up in the atmosphere (see Section 6.2.3). Many fluorinated gases have very high global warming potentials (GWPs) relative to other greenhouse gases, so small atmospheric concentrations can have disproportionately large effects on global temperatures (US EPA, 2022cw).

The GWP is defined by the Intergovernmental Panel on Climate Change (IPCC, 2014) as *“an index measuring the radiative forcing following an emission of a unit mass of a given substance, accumulated over a chosen time horizon, relative to that of the reference substance, carbon dioxide (CO_2). The GWP thus represents the combined effect of the* *differing times these substances remain in the atmosphere and their effectiveness in causing radiative forcing."*

In 2010, fluorinated gases covered under the Kyoto Protocol (F-gases) accounted for 2% of total anthropogenic greenhouse gas emissions (IPCC, 2014) and PFCs contribute to this.

Greenhouse gas emissions for PFCs are quantified as CO_2-equivalent emissions (in gigatonnes) ($GtCO_2$-eq) using weightings based on the energy absorbed by a gas over 100 years (the 100-year GWP). PFBE is not listed in IPCC (2013) as it is not a gas. However, PFBE is listed in the US EPA Greenhouse Gas Reporting Programme as having a 100-year GWP of 0.16 $GtCO_2$-eq (US EPA, 2017; substance listed as Capstone 42-U, CAS 19430-93-4). On the basis of the value reported by US EPA (2017) PFBE might make a contribution to global warming.

9.6 Limit values

9.6.1 Predicted No Effect Concentration (PNEC) derivation

A PNEC is an indication of an acceptable environmental concentration based on evidence from toxicity studies. Available hazard data are discussed in Sections 7 and 8. No PNEC values were presented in the EU REACH registration dossier. PNECs have also been derived by the Environment Agency following REACH guidance (ECHA, 2008) and are shown in Table 9.1. Due to the lack of effects observed in the acute ecotoxicity studies, a reliable aquatic PNEC cannot be estimated. ECHA (2008) states that a long-term test (on invertebrates, preferably *Daphnia*) has to be carried out for substances showing no toxicity in short-term tests if the log $K_{OW} > 3$ (or BCF > 100) and if the Predicted Environmental Concentration (PEC) local or regional is greater than 1/100th of the water solubility (>0.015 mg/L in this case). This is effectively a screening PNEC and so has been used here to give an indication of whether additional chronic ecotoxicity testing may be required. Due to the lack of a reliable aquatic PNEC, soil and sediment PNECs have not been calculated based on the Equilibrium Partitioning Method (EPM) at this time.

Table 9.1 PNECs derived for PFBE by the Environment Agency

Protection goal	Most sensitive toxicity descriptor	Assessment factor	PNEC	Justification/ remarks
Fresh surface water	-	-	0.015 mg/L	A reliable PNEC cannot be estimated based on the currently available ecotoxicity data set. A screening PNEC of 1/100th water solubility is used to indicate whether chronic ecotoxicity data is required.
Freshwater sediment				Not calculated
Sewage treatment micro-organisms				No sludge respiration EC_{10} or NOEC available.
Marine surface water				Not calculated
Marine sediment				Not calculated
Soil				Not calculated
Secondary poisoning				Not calculated

9.6.2 Qualitative/semi-quantitative descriptors for other critical hazards

PFBE smeets the vPvM screening criteria, although it is a volatile liquid. The UK Government has not yet taken a position on whether or how to manage emissions of potential PMT/vPvM substances, and so this will need to be reconsidered once a policy position has been adopted.

As noted in Section 9.5, PFBE may contribute to global warming, which could be considered a qualitative hazard.

10 Exposure assessment

10.1 Environment

10.1.1 Environmental releases

The information in this section is based on the Chemical Safety Report (CSR) submitted by the lead Registrant to ECHA when the UK was still a member of the EU, supplemented with other information from further dialogue with the UK importer. Most of the available information is confidential, so only a summary is presented here.

PFBE is used as a co-monomer in the production of both ETFE and PTFE. Releases of PFBE occur to air and trace amounts to water during the manufacture of fluoropolymers.

Both PTFE and ETFE have a wide variety of uses in industrial processes (e.g. in the semi-conductor industry, in cable coating, in the automotive industry and architecture). PFBE is unlikely to be present as an impurity in the final consumer or industrial product of PTFE but could be present in trace amounts in ETFE. Environmental releases may therefore occur to wastewater and air during the processing and use of ETFE.

10.1.2 Exposure scenarios and measures for reducing emissions to the environment

10.1.2.1 Polymer manufacture

PFBE is manufactured in Japan and imported to a single site in the UK (AGC Chemicals Europe Ltd, Fleetwood Road North, Thornton Cleveleys, Lancashire FY5 4QD).

PFBE is used at this site as a co-monomer for the manufacture of ETFE and co-monomer in PTFE production. This involves two separate production plants. PFBE is received in sealed containers, pumped into storage tanks and then transferred as necessary to the reactors. Sampling for quality control is not undertaken on the site.

In the ETFE process when the batch reaction in the reactor is complete, the ETFE slurry is dried and the water / solvent mix containing PFBE is driven off in a number of heating steps to recover and distil the solvent, which contains trace quantities of PFBE for reuse. The remaining water from this heating process is released as wastewater. In the PTFE process, most of the PFBE is used up in the reaction, but a very small quantity could be released to air at the end of each batch when the reactor vessel is purged although the majority of the purge gas is captured.

The company has an environmental permit (ref: EPR/BU5453IY) under the Environmental Permitting (England and Wales) Regulations 2016. According to the permit, the fluoropolymer production capacity is 6 000 tonnes/year. The permit does not require any monitoring for PFBE or require any specific control measures. The company undertook a mass balance calculation for each of the manufacturing lines and provided these for the evaluation.

Routes of emission to surface water

The wastewater from the recovery processes in the ETFE production line, along with wastewater from other processes on site, drains to the waste effluent pit, which goes to the clarifiers to remove solids and is then discharged to the River Wyre. This process is not designed to remove PFBE. AGC Chemicals Europe Ltd estimate an annual release of less than 1 kg/year PFBE, based on the mass balance.

Given this small amount of release, and the dilution provided by the River Wyre, the Environment Agency has not performed any modelling to derive a predicted environmental concentration (PEC).

Routes of emission to land

There is no direct emission to land from the site, and since the wastewater is not treated in a municipal sewage treatment plant (STP), it is not present in sewage sludge that can be spread on agricultural land.

Routes of emission to air

The main release point is in the recovery process in the ETFE production plant. Gaseous PFBE from ETFE process is captured in solvent-laden-gas (SLG) recovery system by activated carbon bed and recovered back to the process as liquid. Releases to air occur from carbon adsorption unit which is a permitted emission point. AGC Chemicals Europe Ltd estimates a total annual PFBE release from all on-site release points of less than 900 kg/year, based on a mass balance undertaken each year.

In the mass balance for PTFE, the company calculates that all the PFBE is consumed in the polymerisation process, but as a worst case have estimated a release to air of 0.5 kg/year (N.B. this is for all markets, not just the UK).

Since distribution modelling suggests that any substance released to air will remain there (see Section 6.2.3), the Environment Agency has not performed any modelling to derive PECs for environmental media.

10.1.3 Polymer use

The quantity of PFBE in the ETFE products supplied to customers is <0.5 kg/year (N.B. this is for all markets, not just the UK). This is based on the mass balance and an extrapolation from estimates of process solvent levels in the final polymer. PFBE is estimated to be present at approximately 0.5% in this solvent.

In their mass balance calculations for the PTFE process, the company estimates that all of the PFBE is used up in the reaction and that there would be no residual monomer in the final polymer product.

10.1.4 Monitoring data

The company has not undertaken any monitoring for releases of PFBE to either wastewater or the atmosphere.

11 Risk characterisation

Environmental releases from the UK manufacturing site are expected to be less than 900 kg/year to air and less than 1 kg/year to water. A reasonable worst-case estimate is that the residual PFBE content in polymers on the UK market (from all suppliers) will be lower than 0.5 kg/year.

No significant adverse effects have been observed in the available aquatic ecotoxicity studies, although long-term data for fish and invertebrates are not available. Since the substance is not rapidly degradable, and it has a log K_{OW} above 4, it is proposed that it should be self-classified as Aquatic Chronic 4. Although aquatic PNECs have been derived, they are screening values based on the water solubility. The substance does not meet the PBT/vPvB or draft PMT criteria but does screen as potentially meeting the draft vPvM criteria and no information is available about endocrine disruption.

On the basis of low releases and lack of significant adverse effects in the information currently available, the Environment Agency considers that the direct risk to the environment from PFBE is likely to be low.

A conclusion cannot be drawn about risks arising from the vPvM properties of the substance until a UK Government policy position is available. However, aquatic emissions are very low. The influence of volatility is also not considered under the criteria.

PFBE might contribute to global warming. The Environment Agency recommends that this should be considered as part of any emission controls.

12 Conclusions and recommendations

12.1 Conclusion

PFBE is a PFAS that belongs to the HFC group. It is imported to the UK and used as a co-monomer to manufacture fluorinated polymers at a single site. A low level of release occurs to air during the manufacture of fluoropolymers at this site, and there is also likely to be release of smaller quantities to the River Wyre. Very small releases may also occur at polymer processing sites. PFBE is volatile and is expected to partition significantly to the atmosphere. It may have the potential to be transported to remote regions.

Based on the available hazard data the following conclusions can be reached:

- PFBE meets the criteria to be classified as Aquatic Chronic 4 for aquatic environmental hazard under CLP legislation but does not meet the T criterion of REACH Annex 13.
- PFBE is not readily biodegradable and is not expected to degrade abiotically. PFBE therefore screens as potentially persistent or very persistent.
- The log K_{OW} and log K_{OA} indicate that the substance does not meet the REACH Annex 13 bioaccumulation screening criteria.
- PFBE is unlikely to be PBT or vPvB, but does meet the draft vPvM criteria. A conclusion cannot be drawn about risks arising from the vPvM properties of the substance until a UK Government policy position is available. However, aquatic emissions are very low. The influence of volatility is not considered under these criteria.
- On the basis of low releases and lack of significant adverse effects according to the information currently available, the Environment Agency considers that the direct risk to the environment from PFBE is likely to be low.
- PFBE might contribute to global warming. In addition, no data about biotic effects (e.g. to plants) from aerial exposure are available.
- PFBE is likely to be a source of perfluoropentanoic acid and perfluorobutanoic acid in the environment. An assessment of their properties (and other contributing substances) is outside scope of this evaluation. However, they are both likely to be vPvM, and so PFBE would be relevant in terms of any risk management associated with these “arrowhead” substances.

12.2 Recommendations

12.2.1 Recommendations to the UK supplier

Although this evaluation is not a formal assessment under UK REACH, the Environment Agency proposes several ways to improve the data package to allow a more robust assessment of the hazards and risks posed by PFBE, including:

- A self-classification of Aquatic Chronic 4 for aquatic environmental hazard under the CLP legislation, which in turn would trigger an exposure assessment; and
- Justification for the atmospheric half-life of 6.4 hours stated in the PBT assessment of the EU REACH registration dossier, as well as information on likely transformation products.

PFBE is expected to partition to the atmosphere and could contribute to global warming. The UK supplier is invited to consider this as part of any voluntary action it may take to improve emission controls.

12.2.2 General regulatory recommendations for consideration by relevant UK authorities

The Environment Agency along with HSE have been undertaking a Regulatory Management Options Analysis (RMOA) for PFAS, and the information summarised in this evaluation has fed into that analysis to identify the most appropriate risk management measures for PFAS in a UK context.

13 References

Arp, H.P. and Hale, S.E., 2019. REACH: Improvement of guidance and methods for the identification and assessment of PMT/vPvM substances. Wörlitzer: Umweltbundesamt.

ECHA, 2008. Guidance on information requirements and chemical safety assessment: Chapter R.10: Characterisation of dose [concentration]-response for environment [online]. Helsinki: European Chemicals Agency. https://echa.europa.eu/documents/10162/13632/information_requirements_r10_en.pdf/bb902be7-a503-4ab7-9036-d866b8ddce69 (Accessed March 2022).

ECHA 2011. Guidance on Information Requirements and Chemical Safety Assessment. Chapter R.4: Evaluation of Available Information. Versions 1.1. December 2011. European Chemicals Agency, Helsinki, Finland. https://echa.europa.eu/documents/10162/13643/information_requirements_r4_en.pdf/d6395ad2-1596-4708-ba86-0136686d205e (Accessed March 2022)

ECHA 2016a. Guidance on Information Requirements and Chemical Safety Assessment. Chapter R.16: Environmental Exposure Assessment. Versions 3.0. February 2016. European Chemicals Agency, Helsinki, Finland. https://echa.europa.eu/documents/10162/13632/information_requirements_r16_en.pdf (Accessed March 2022)

ECHA (2017c). Guidance on Information Requirements and Chemical Safety Assessment. Chapter R.7c: Endpoint Specific Guidance. Versions 3.0. June 2017. European Chemicals Agency, Helsinki, Finland. https://echa.europa.eu/documents/10162/13632/information_requirements_r7c_en.pdf

ECHA, 2017d. Read-Across Assessment Framework (RAAF). European Chemicals Agency, Helsinki, Finland. https://echa.europa.eu/documents/10162/13628/raaf_en.pdf/614e5d61-891d-4154-8a47-87efebd1851a

ECHA, 2019. EUSES - European Union System for the Evaluation of Substances. Version 2.2.0. https://echa.europa.eu/support/dossier-submission-tools/euses.

ECHA, 2020. ECHA Registered Substances. European Chemicals Agency, Helsinki, Finland. https://echa.europa.eu/information-on-chemicals/registered-substances (Accessed July 2020)

ECHA, 2022a. European Chemicals Agency, Helsinki, Finland. https://echa.europa.eu/registration-dossier/-/registered-dossier/5646/ (Accessed March 2022)

ECHA, 2022b. Summary of Classification and Labelling for PFBE. Helsinki: European Chemicals Agency. https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/15890. (Accessed March 2022).

ECHA, 2022c. European Chemicals Agency, Helsinki, Finland. https://echa.europa.eu/substance-information/-/substanceinfo/100.015.717 (Accessed March 2022)

ECHA, 2022d. European Chemicals Agency, Helsinki, Finland. https://echa.europa.eu/substance-information/-/substanceinfo/100.042.523 (Accessed March 2022)

ECHA, 2022e. European Chemicals Agency, Helsinki, Finland. https://echa.europa.eu/registration-dossier/-/registered-dossier/27020 (Accessed June 2022)

Environment Canada (2012). Ecological Screening Assessment Report. Long-Chain (C9-C20) Perfluorocarboxylic Acids, their Salts and their Precursors.

Gomis, M.I., Wang, Z., Scheringer, M. and Cousins, I.T. 2015. A modelling assessment of the physicochemical properties and environmental fate of emerging and novel per- and polyfluoroalkyl substances. Science of the Total Environment, 505, 981-991.

IPCC, 2013. Myhre, G., D. Shindell, F.-M. Bréon, W. Collins, J. Fuglestvedt, J. Huang, D. Koch, J.-F. Lamarque, D. Lee, B. Mendoza, T. Nakajima, A. Robock, G. Stephens, T. Takemura and H. Zhang, 2013: Anthropogenic and Natural Radiative Forcing. In: Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change [Stocker, T.F., D. Qin, G.-K. Plattner, M. Tignor, S.K. Allen, J. Boschung, A. Nauels, Y. Xia, V. Bex and P.M. Midgley (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA.
https://www.ipcc.ch/pdf/assessmentreport/ar5/wg1/WG1AR5_Chapter08_FINAL.pdf

IPCC, 2014. Climate Change 2014: Synthesis report. Contribution of Working Groups I, II and III to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change [Core writing team, R.K. Pachauri and L.A. Meyer (eds)]. IPCC, Geneva, Switzerland.

Mansouri, K., Grulke, C.M., Richard, A.M., Judson, R.S. and Williams, A.J. 2016. An automated curation procedure for addressing chemical errors and inconsistencies in public datasets used in QSAR modelling. SAR and QSAR in Environmental Research, 27(11), 911-937.

Mansouri, K. Grulke, C., Judson, R., Williams, A. 2018. OPERA: A free and open source QSAR tool for predicting physicochemical properties and environmental fate endpoints. Abst. Papers Am. Chem. Soc. p. 255.

NCBI, 2022 National Center for Biotechnology Information. "PubChem Compound Summary for CID 88054, 3,3,4,4,5,5,6,6,6-Nonafluoro-1-hexene" PubChem, https://pubchem.ncbi.nlm.nih.gov/compound/Perfluorobutyl_ethylene (Accessed March 2022).

OECD, 1981. Test No. 305C: Degree of bioconcentration in fish, Section 3, OECD Publishing Paris.

OECD, 1992. Environment Monograph No. 61. The Rate of Photochemical Transformation of Gaseous Organic Compounds in Air under Tropospheric Conditions. OCDE/GD(92)172. https://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?doclanguage=en&cote=ocde/gd(92)172

OECD, 1995a. Test No. 105: Water Solubility, OECD Guidelines for the Testing of Chemicals, Section 1, OECD Publishing, Paris. https://doi.org/10.1787/9789264069589-en (Accessed July, 2020)

OECD, 1995b. Test No. 107: Partition Coefficient (n-octanol/water): Shake Flask Method, OECD Guidelines for the Testing of Chemicals, Section 1, OECD Publishing, Paris, https://doi.org/10.1787/9789264069626-en (Accessed July, 2020)

OECD, 2004. Test No. 117: Partition Coefficient (n-octanol/water), HPLC Method, OECD Guidelines for the Testing of Chemicals, Section 1, OECD Publishing, Paris, https://doi.org/10.1787/20745753 (Accessed July, 2020)

OECD, 2006a. Test No. 104: Vapour Pressure, OECD Guidelines for the Testing of Chemicals, Section 1, OECD Publishing, Paris, https://doi.org/10.1787/20745753

OECD, 2006b. Test No. 123: Partition Coefficient (1-Octanol/Water): Slow-Stirring Method, OECD Guidelines for the Testing of Chemicals, Section 1, OECD Publishing, Paris, https://doi.org/10.1787/9789264015845-en (Accessed July, 2020)

OECD (2000), Test No. 106: Adsorption -- Desorption Using a Batch Equilibrium Method, OECD Guidelines for the Testing of Chemicals, Section 1, OECD Publishing, Paris, https://doi.org/10.1787/9789264069602-en (Accessed December 2021)

OECD, 2012. Test No. 305: Bioaccumulation in Fish: Aqueous and Dietary Exposure. OECD Guidelines for the Testing of Chemicals, Section 3, OECD Publishing, Paris https://www.oecd-ilibrary.org/environment/test-no-305-bioaccumulation-in-fish-aqueous-and-dietary-exposure_9789264185296-en (Accessed July, 2020)

OECD, 1992. Test No. 301D. Ready biodegradability. https://www.oecd-ilibrary.org/environment/test-no-301-ready-biodegradability_9789264070349-en (Accessed March 2022)

OECD, 2001. Test No. 121. Estimation of the Adsorption Coefficient (K_{oc}) on Soil and on Sewage Sludge using High Performance Liquid Chromatography (HPLC).

https://www.oecd-ilibrary.org/environment/test-no-121-estimation-of-the-adsorption-coefficient-koc-on-soil-and-on-sewage-sludge-using-high-performance-liquid-chromatography-hplc_9789264069909-en (Accessed March 2022)

OECD, 2019. Test No. 203. Fish, Acute Toxicity Test. https://www.oecd-ilibrary.org/environment/test-no-203-fish-acute-toxicity-test_9789264069961-en (Accessed March 2022)

OECD, 2004. Test No. 202. Daphnia sp. Acute Immobilisation Test. https://www.oecd-ilibrary.org/environment/test-no-202-daphnia-sp-acute-immobilisation-test_9789264069947-en (Accessed March 2022

OECD, 2011. Test No. 201. Freshwater Alga and Cyanobacteria, Growth Inhibition Test. https://www.oecd-ilibrary.org/environment/test-no-201-alga-growth-inhibition-test_9789264069923-en (Accessed March 2022

OECD, 2018a. Test No. 412. Subacute Inhalation Toxicity: 28-Day Study. https://www.oecd-ilibrary.org/environment/test-no-412-subacute-inhalation-toxicity-28-day-study_9789264070783-en (Accessed March 2022)

OECD, 2018b. Test No. 413. Subchronic Inhalation Toxicity: 90-day Study. https://www.oecd-ilibrary.org/environment/test-no-413-subchronic-inhalation-toxicity-90-day-study_9789264070806-en (Accessed March 2022)

OECD, 2018c. Test No. 414. Prenatal Developmental Toxicity Study. https://www.oecd-ilibrary.org/environment/test-no-414-prenatal-development-toxicity-study_9789264070820-en (Accessed March 2022)

OECD, 2019. Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures, OECD Series on Testing and Assessment, OECD Publishing, Paris, https://doi.org/10.1787/0ed2f88e-en.

RSC, 2022. Royal Society of Chemistry. ChemSpider. [ONLINE]. Version 2020.0.18.0. http://www.chemspider.com/Chemical-Structure.61049.html (Accessed March 2022)

Unpublished. 1980. Unpublished. Cited in ECHA, 2022a

Unpublished. 1981. Unpublished. Cited in ECHA, 2022a

Unpublished, 2001. Unpublished. Cited in ECHA, 2022a

Unpublished, 2010. Unpublished. Cited in ECHA, 2022a.

Unpublished, 2017. Unpublished. Cited in ECHA, 2022a.

US EPA, 2012. EPISuite^{TM} v4.11. United States Environmental Protection Agency Office of Pollution Prevention Toxics and Syracuse Research Corporation.

US EPA, 2016. User's Guide for T.E.S.T. (Toxicity Estimation Software Tool), EPA/600/R-16/058, United States Environmental Protection Agency, Washington, DC, USA [online]. https://www.epa.gov/sites/production/files/2016-05/documents/600r16058.pdf (Accessed July 2020).

US EPA, 2017. Greenhouse Gas Reporting Program: Addition of Global Warming Potentials to the General Provisions and Amendments and Confidentiality Determinations for Fluorinated Gas Production. https://www.govinfo.gov/content/pkg/CFR-2017-title40-vol23/xml/CFR-2017-title40-vol23-part98-subpartA-appA.xml (Accessed September 2022).

US EPA, 2020. Assessing and Managing Chemicals Under TSCA. Low-priority Substances Under TSCA [online]. United States Environmental Protection Agency, Washington DC, USA. https://www.epa.gov/assessing-and-managing-chemicals-under-tsca/low-priority-substances-under-tsca (Accessed July 2020

US EPA, 2022a. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/chemical/details/DTXSID6047575 (Accessed March 2022)

US EPA, 2022b. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID10232971 (Accessed March 2022)

US EPA, 2022c. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID8067076 (Accessed March 2022)

US EPA CompTox 2022d. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID90180087 (Accessed March 2022)

US EPA CompTox 2022e. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID7074616 (Accessed March 2022)

US EPA CompTox 2022f. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID40895311 (Accessed March 2022)

US EPA CompTox 2022g. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].

https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID60184471 (Accessed March 2022)

US EPA CompTox 2022h. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID40895376 (Accessed March 2022)

US EPA CompTox 2022i. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID20382072 (Accessed March 2022)

US EPA CompTox 2022j. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID80895451 (Accessed March 2022)

US EPA CompTox 2022k. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID40895472 (Accessed March 2022)

US EPA CompTox 2022l. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID40895154 (Accessed March 2022)

US EPA CompTox 2022m. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID80880145 (Accessed March 2022)

US EPA CompTox 2022n. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID20170895 (Accessed March 2022)

US EPA CompTox 2022o. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID90371872 (Accessed March 2022)

US EPA CompTox 2022p. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].

https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID10379279 (Accessed March 2022)

US EPA CompTox 2022q. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID70896659 (Accessed March 2022)

US EPA CompTox 2022r. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID00896662 (Accessed March 2022)

US EPA CompTox 2022s. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID10895242 (Accessed March 2022)

US EPA CompTox 2022t. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID40895235 (Accessed March 2022)

US EPA CompTox 2022u. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID20896664 (Accessed March 2022)

US EPA CompTox 2022v. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID80896665 (Accessed March 2022)

US EPA CompTox 2022w. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID20379927 (Accessed March 2022)

US EPA CompTox 2022x. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID40896762 (Accessed March 2022)

US EPA CompTox 2022y. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].

https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID90895285 (Accessed March 2022)

US EPA CompTox 2022z. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID30895300 (Accessed March 2022)

US EPA CompTox 2022aa. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID40895295 (Accessed March 2022)

US EPA CompTox 2022ab. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID60896668 (Accessed March 2022)

US EPA CompTox 2022ac. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID20895339 (Accessed March 2022)

US EPA CompTox 2022ad. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID60895338 (Accessed March 2022)

US EPA CompTox 2022ae. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID30895340 (Accessed March 2022)

US EPA CompTox 2022af. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID80895350 (Accessed March 2022)

US EPA CompTox 2022ag. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID60895373 (Accessed March 2022)

US EPA CompTox 2022ah. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].

https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID70895389
(Accessed March 2022)

US EPA CompTox 2022ai. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].
https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID10895429
(Accessed March 2022)

US EPA CompTox 2022aj. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].
https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID90895422
(Accessed March 2022)

US EPA CompTox 2022ak. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].
https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID10379855
(Accessed March 2022)

US EPA CompTox 2022al. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].
https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID70895440
(Accessed March 2022)

US EPA CompTox 2022am. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].
https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID60709981
(Accessed March 2022)

US EPA CompTox 2022an. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].
https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID60895419
(Accessed March 2022)

US EPA CompTox 2022ao. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].
https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID20895415
(Accessed March 2022)

US EPA CompTox 2022ap. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].
https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID10895409
(Accessed March 2022)

US EPA CompTox 2022aq. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].

https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID10895444 (Accessed March 2022)

US EPA CompTox 2022ar. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID50896677 (Accessed March 2022)

US EPA CompTox 2022as. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID00707966 (Accessed March 2022)

US EPA CompTox 2022at. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID30895461 (Accessed March 2022)

US EPA CompTox 2022au. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID70895485 (Accessed March 2022)

US EPA CompTox 2022av. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID90895462 (Accessed March 2022)

US EPA CompTox 2022aw. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID70895460 (Accessed March 2022)

US EPA CompTox 2022ax. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID50895504 (Accessed March 2022)

US EPA CompTox 2022ay. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID70895465 (Accessed March 2022)

US EPA CompTox 2022az. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].

https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID30896675 (Accessed March 2022)

US EPA CompTox 2022ba. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID40895518 (Accessed March 2022)

US EPA CompTox 2022bb. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID80896680 (Accessed March 2022)

US EPA CompTox 2022bc. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID10896678 (Accessed March 2022)

US EPA CompTox 2022bd. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID60896683 (Accessed March 2022)

US EPA CompTox 2022be. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID30895527 (Accessed March 2022)

US EPA CompTox 2022bf. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID20895551 (Accessed March 2022)

US EPA CompTox 2022bg. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID40880444 (Accessed March 2022)

US EPA CompTox 2022bh. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID20896684 (Accessed March 2022)

US EPA CompTox 2022bi. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].

https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID60895530 (Accessed March 2022)

US EPA CompTox 2022bj. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID70895566 (Accessed March 2022)

US EPA CompTox 2022bk. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID00895574 (Accessed March 2022)

US EPA CompTox 2022bl. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID40896686 (Accessed March 2022)

US EPA CompTox 2022bm. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID00896687 (Accessed March 2022)

US EPA CompTox 2022bn. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID70895602 (Accessed March 2022)

US EPA CompTox 2022bo. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID50896692 (Accessed March 2022)

US EPA CompTox 2022bp. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID30503716 (Accessed March 2022)

US EPA CompTox 2022bq. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID50895180 (Accessed March 2022)

US EPA CompTox 2022br. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].

https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID90455222 (Accessed March 2022)

US EPA CompTox 2022bs. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID80454860 (Accessed March 2022)

US EPA CompTox 2022bt. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID80895193 (Accessed March 2022)

US EPA CompTox 2022bu. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID10711635 (Accessed March 2022)

US EPA CompTox 2022bv. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID70379270 (Accessed March 2022)

US EPA CompTox 2022bw. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID60895171 (Accessed March 2022)

US EPA CompTox 2022bx. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID30895183 (Accessed March 2022)

US EPA CompTox 2022by. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID90895189 (Accessed March 2022)

US EPA CompTox 2022bz. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID80896660 (Accessed March 2022)

US EPA CompTox 2022ca. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].

https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID00895231 (Accessed March 2022)

US EPA CompTox 2022cb. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID30709115 (Accessed March 2022)

US EPA CompTox 2022cc. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID40896666 (Accessed March 2022)

US EPA CompTox 2022cd. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID60345848 (Accessed March 2022)

US EPA CompTox 2022ce. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID50896672 (Accessed March 2022)

US EPA CompTox 2022cf. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID90764184 (Accessed March 2022)

US EPA CompTox 2022cg. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID60346052 (Accessed March 2022)

US EPA CompTox 2022ch. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID90895306 (Accessed March 2022)

US EPA CompTox 2022ci. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID80447691 (Accessed March 2022)

US EPA CompTox 2022cj. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].

https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID90848135 (Accessed March 2022)

US EPA CompTox 2022ck. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID80190837 (Accessed March 2022)

US EPA CompTox 2022cl. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID70170108 (Accessed March 2022)

US EPA CompTox 2022cm. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID00600903 (Accessed March 2022)

US EPA CompTox 2022cn. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID50603909 (Accessed March 2022)

US EPA CompTox 2022co. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID00380854 (Accessed March 2022)

US EPA CompTox 2022cp. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID10896658 (Accessed March 2022)

US EPA CompTox 2022cq. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID00346051 (Accessed March 2022)

US EPA CompTox 2022cr. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID80622108 (Accessed March 2022)

US EPA CompTox 2022cs. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE].

https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID50449869 (Accessed March 2022)

US EPA CompTox 2022ct. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID10461880 (Accessed March 2022)

US EPA CompTox 2022cu. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID80228205 (Accessed March 2022)

US EPA CompTox 2022cv. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. [ONLINE]. https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID90379833 (Accessed March 2022)

US EPA, 2022cw. Greenhouse Gas Emissions [ONLINE] U.S. Environmental Protection Agency, Washington, DC. https://www.epa.gov/ghgemissions/overview-greenhouse-gases#f-gases (Accessed March 2022)

US EPA, 2022cx. U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. https://comptox.epa.gov/dashboard/DTXSID2026949 (accessed March 2022).

US EPA, 2022cy. U.S. Environmental Protection Agency. Product Properties Test Guidelines: OPPTS 830.7840 Water Solubility: Column Elution Method; Shake Flask Method [EPA 712–C–98–041], March 1998.

US EPA, 2022cz. U.S. Environmental Protection Agency. Product Properties Test Guidelines: OPPTS 830.7550 Partition Coefficient (n-Octanol/Water), Shake Flask Method [EPA 712–C–96–038], August 1996.

US EPA, 2022da. PFAS Analytical Methods Development and Sampling Research. https://www.epa.gov/water-research/pfas-analytical-methods-development-and-sampling-research (Accessed March 2022)

Wegmann, Cavin, MacLeod, Scheringer and Hungerbühler, 2009. The OECD software tool for screening chemicals for persistence and long-range transport potential. Environmental Modeling and Software, 24, 228-237.

Williams, A.J., Grulke, C.M., Edwards, J. 2017. The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. J. Cheminform., 9, 61. https://doi.org/10.1186/s13321-017-0247-6 (Accessed July 2020)

14 List of abbreviations

%	Percentage
B	Bioaccumulative
BAF	Bioaccumulation factor
BCF	Bioconcentration factor
BMF	Biomagnification factor
CAS	Chemical Abstracts Service
CLP	Classification, labelling and packaging (of substances and mixtures)
cm	Centimetre
CoRAP	Community Rolling Action Plan
CSR	Chemical Safety Report
d	Day
DegT$_{50}$	Degradation half-life or transformation half-life (days)
DMEL	Derived Minimal Effect Level
DNEL	Derived No Effect Level
DSD	Dangerous Substances Directive
DT$_{50}$	Dissipation half-life (days)
dw	Dry weight
EC$_{10}$	10% effect concentration
EC$_{50}$	50% effect concentration
ELR50	50% effect loading rate
ECETOC TRA	European Centre for Ecotoxicology and Toxicology of Chemicals Targeted Risk Assessment
ECHA	European Chemicals Agency
EPA	Environmental Protection Agency

EPM	Equilibrium Partitioning Method
EQS	Environmental Quality Standard
ERC	Environmental release category
ES	Exposure Scenario
EU	European Union
EUSES	European Union System for the Evaluation of Substances
FSDT	Fish Sexual Development Test
g	Gramme
GC	Gas chromatography
GC/FID	Gas chromatography – Flame Ionisation Detection
GC/MS	Gas chromatography – mass spectrometry
GLP	Good laboratory practice
H	Hours
HLC	Henry's Law Constant
hPa	Hectopascal
HPLC	High performance liquid chromatography
HSE	Health and Safety Executive
ISO	International Organisation for Standardisation
IUCLID	International Uniform Chemical Information Database
IUPAC	International Union of Pure and Applied Chemistry
kg	Kilogram
kJ	Kilojoule
km	Kilometre
K_{AW}	Air-water partition coefficient
K_{OA}	Octanol-air partition coefficient

K_{OC}	Organic carbon-water partition coefficient
K_{OW}	Octanol-water partition coefficient
kPa	Kilopascal
$K_{SUSP–WATER}$	Suspended matter–water partitioning coefficient
k_X	Rate constants (days-1)
L	Litre
LC_{50}	50% lethal effect concentration
LEV	Local Exhaust Ventilation
LOD	Limit of detection
Log	Logarithmic value
LOQ	Limit of quantitation
M	Molar
m/z	Mass to charge ratio
mg	Milligram
min	Minute
mL	Millilitre
mol	Mole
MS	Mass spectrometry
nm	Nanometre
NOAEL	No observed adverse effect level
NOEC	No-observed effect concentration
NOEL	No observed effect level
NONS	Notification of New Substances Regulations 1993
OC	Operational condition
OECD	Organisation for Economic Co-operation and Development

OSPAR	Oslo and Paris Convention for the Protection of the Marine Environment of the North-East Atlantic
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
p	Statistical probability
Pa	Pascal
PACT	Public Activities Co-ordination Tool
PBT	Persistent, Bioaccumulative and Toxic
PC	Product category
PEC	Predicted environmental concentration
pg	Picogramme
PFAS	Per- and polyfluorinated alkyl substances
PFOS	Perfluorooctanesulfonate
PFOA	Perfluorooctanoic acid
pKa	Acid dissociation constant
PNEC	Predicted no effect concentration
POP	Persistent organic pollutant
ppb	Parts per billion
PPE	Personal Protective Equipment
ppm	Parts per million
PROC	Process Category
QSAR	Quantitative structure-activity relationship
OPERA	OPEn structure–activity/property Relationship App
r^2	Correlation coefficient
RCR	Risk characterisation ratio
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals (EU Regulation No. 1907/2006)

RMM	Risk Management Measures
RPE	Respiratory protective equipment
rpm	Revolutions per minute
SMILES	Simplified Molecular Input Line Entry System
SVHC	Substance of Very High Concern
t	Tonne
T.E.S.T	Toxicity Estimation Software Tool
TG	Test Guideline
TMF	Trophic Magnification Factor
TSCA	Toxic Substances Control Act
UNEP	United Nations Environment Programme
UK	United Kingdom
US EPA	United Stated Environmental Protection Agency
UV	Ultraviolet
vB	Very bioaccumulative
vP	Very persistent
VP	Vapour pressure
vPvB	Very persistent and very bioaccumulative
WAF	Water Accommodated Fraction
WSF	Water Soluble Fraction
wt	Weight
ww	Wet weight
WWTP	Wastewater Treatment Plant
µg	Microgram

Appendix A: Literature search

A literature search was undertaken by the Environment Agency on the 8th April 2020 to identify published information relevant to the assessment of PFBE. The keywords listed in Table 10 were searched for in PubMed (https://pubmed.ncbi.nlm.nih.gov/) and Science Direct (https://www.sciencedirect.com/). In order to maximise the number of records identified keywords were based on the substance name only, and not on the endpoints of interest or year of publication.

Table A.1 Literature search terms and number of hits

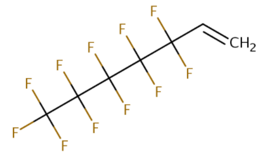
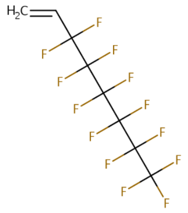
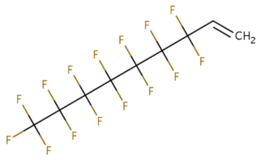
Search terms	PubMed	Science Direct
19430-93-4	5	8
3,3,4,4,5,5,6,6,6-Nonafluorohexene	0	5
3,3,4,4,5,5,6,6,6-nonafluorohex-1-ene	0	2
Perfluorobutyl ethylene	1	28
PFBE AND fluoro	0	5
Total unique records	6	43

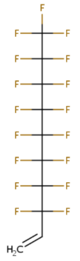
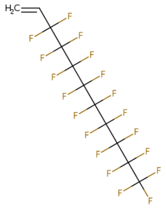
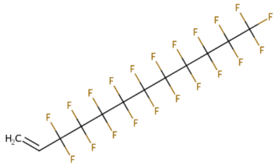
The identified records were screened manually for relevance to this assessment based on the title and abstract. Articles identified as of potential interest were obtained and reviewed for relevance. Those that were found to be relevant are discussed in the appropriate sections of this report.

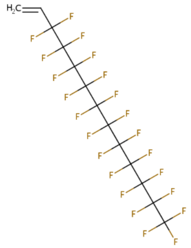
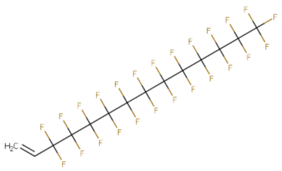
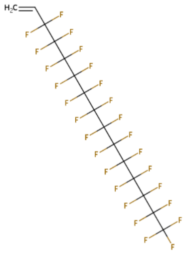
Appendix B: Structural analogues

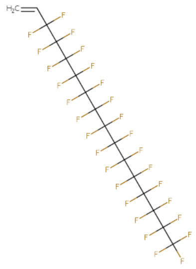
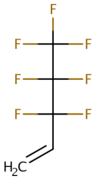
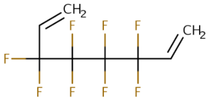
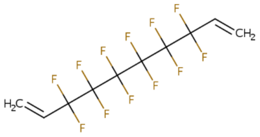
The US EPA CompTox Chemicals database (US EPA, 2022a; accessed March 2022) was used to identify structures with Tanimoto similarity coefficient >0.8. No experimental data were available for any of those included.

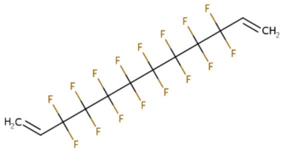
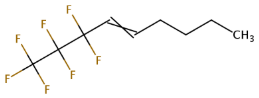
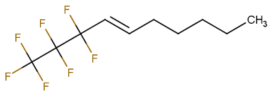
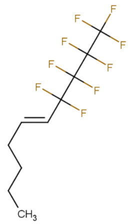
Table B.1 Structural identifiers for analogues of PFBE

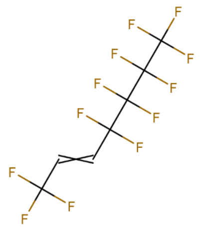
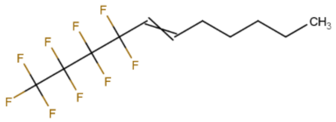
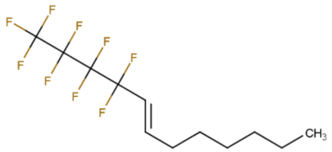
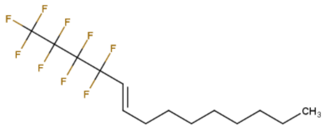
IUPAC name	CAS number	EC number	Structural formula	Molecular formula	Molecular weight (g/mol)	SMILES code	Source
3,3,4,4,5,5,6,6,7,7,7-Undecafluorohept-1-ene	84100-13-0	282-095-0		$C_7H_3F_{11}$	296.083	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=C	US EPA (2022b)
3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooct-1-ene	25291-17-2	246-791-8		$C_8H_3F_{13}$	346.091	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=C	US EPA (2022c)
3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-Pentadecafluoronon-1-ene	25431-45-2	246-976-3		$C_9H_3F_{15}$	396.099	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=C	US EPA (2022d)

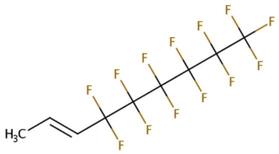
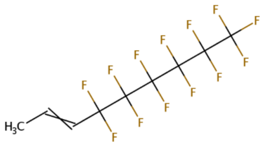
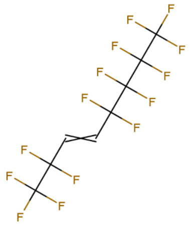
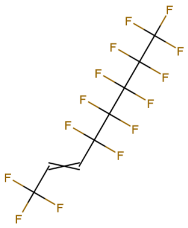
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-Heptadecafluorodec-1-ene	21652-58-4	244-503-5		$C_{10}H_3F_{17}$	446.107	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=C	US EPA (2022e)
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-Nonadecafluoroundec-1-ene	57216-75-8	-		$C_{11}H_3F_{19}$	496.115	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=	US EPA (2022f)
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-Henicosafluorododec-1-ene	30389-25-4	250-173-3		$C_{12}H_3F_{21}$	546.122	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=C	US EPA (2022g)

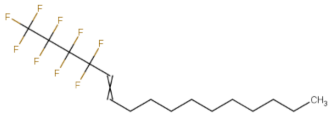
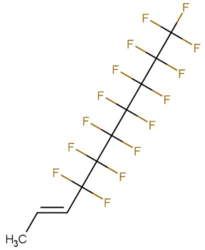
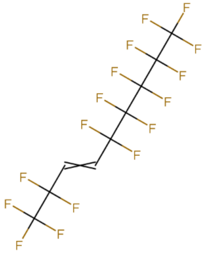
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,13-Tricosafluorotridec-1-ene	1270180-02-3	-		$C_{13}H_3F_{23}$	596.13	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=C	US EPA (2022h)
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-Pentacosafluorotetradec-1-ene	67103-05-3	691-816-1		$C_{14}H_3F_{25}$	646.138	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=C	US EPA (2022i)
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,15,15,15-Heptacosafluoropentadec-1-ene	1270180-04-5	-		$C_{15}H_3F_{27}$	696.146	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=C	US EPA (2022j)

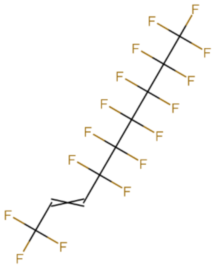
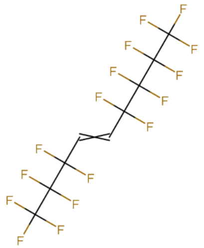
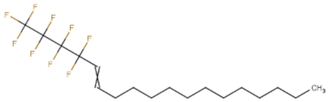
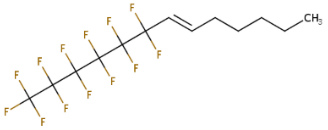
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,15,15,16,16,16-Nonacosafluorohexadec-1-ene	104564-28-5	-		$C_{16}H_3F_{29}$	746.154	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=C	US EPA (2022k)
3,3,4,4,5,5,5-Heptafluoropent-1-ene	355-08-8	206-576-1		$C_5H_3F_7$	196.068	FC(F)(F)C(F)(F)C(F)(F)C=C	US EPA (2022l)
3,3,4,4,5,5,6,6-Octafluoroocta-1,7-diene	678-65-9	211-650-1		$C_8H_6F_8$	254.12	FC(F)(C=C)C(F)(F)C(F)(F)C(F)(F)C=C	US EPA (2022m)
3,3,4,4,5,5,6,6,7,7,8,8-Dodecafluorododeca-1,9-diene	1800-91-5	217-288-0		$C_{10}H_6F_{12}$	354.139	FC(F)(C=C)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=C	US EPA (2022n)

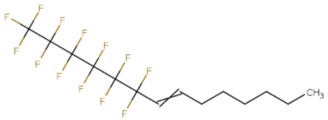
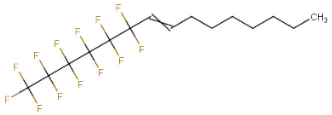
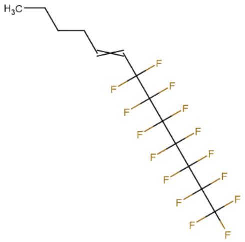
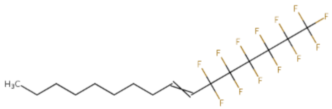
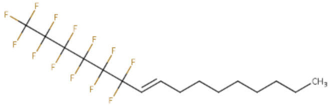
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-Hexadecafluorododeca-1,11-	35192-44-0	671-723-2		$C_{12}H_6F_{16}$	454.154	FC(F)(C=C)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=C	US EPA (2022o)
1,1,1,2,2,3,3-Heptafluoronon-4-ene	57325-40-3	-		$C_9H_{11}F_7$	252.176	CCCCC=CC(F)(F)C(F)(F)C(F)(F)F	US EPA (2022p)
(4E)-1,1,1,2,2,3,3-Heptafluorodec-4-ene	57325-42-5	-		$C_{10}H_{13}F_7$	266.203	CCCCC\C=C\C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022q)
(5E)-1,1,1,2,2,3,3,4,4-Nonafluorodec-5-ene	131294-67-2	-		$C_{10}H_{11}F_9$	302.184	CCCC\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022r)

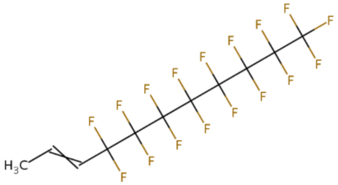
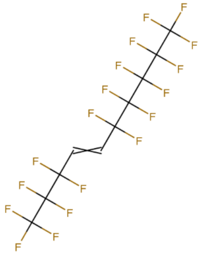
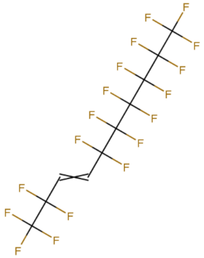
1,1,1,4,4,5,5,6,6,7,7,7-Dodecafluorohept-2-ene	887111-62-8	-		$C_7H_2F_{12}$	314.074	FC(F)(F)C=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022s)
1,1,1,2,2,3,3,4,4-Nonafluoroundec-5-ene	383145-46-8	-		$C_{11}H_{13}F_9$	316.211	CCCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022t)
(5E)-1,1,1,2,2,3,3,4,4-Nonafluorododec-5-ene	113999-54-5	-		$C_{12}H_{15}F_9$	330.238	CCCCCC\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022u)
(5E)-1,1,1,2,2,3,3,4,4-Nonafluorotetradec-5-ene	104504-30-5	-		$C_{14}H_{19}F_9$	358.292	CCCCCCCC\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022v)

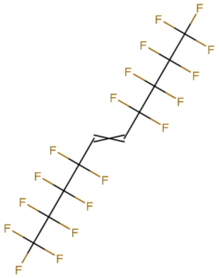
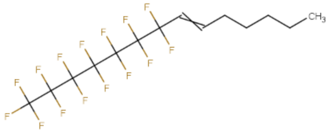
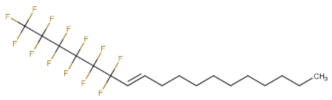
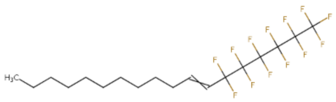
(2E)-4,4,5,5,6,6,7,7,8,8,9,9,9-Tridecafluoronon-2-ene	80793-20-0	-		$C_9H_5F_{13}$	360.118	C\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022w)
4,4,5,5,6,6,7,7,8,8,9,9,9-Tridecafluoronon-2-ene	63967-46-4	-		$C_9H_5F_{13}$	360.118	CC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022x)
1,1,1,2,2,5,5,6,6,7,7,8,8,8-Tetradecafluorooct-3-ene	84808-65-1	-		$C_8H_2F_{14}$	364.082	FC(F)(F)C(F)(F)C=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022y)
1,1,1,4,4,5,5,6,6,7,7,8,8,8-Tetradecafluorooct-2-ene	935476-95-2	-		$C_8H_2F_{14}$	364.082	FC(F)(F)C=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022z)

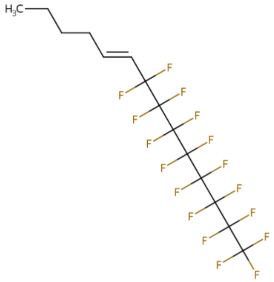
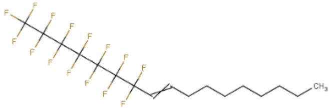
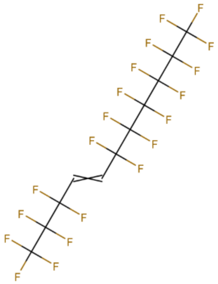
1,1,1,2,2,3,3,4,4-Nonafluorohexadec-5-ene	131851-20-2	-		$C_{16}H_{23}F_9$	386.346	CCCCCCCCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022aa)
(2E)-4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-Pentadecafluorodec-2-ene	89889-22-5	-		$C_{10}H_5F_{15}$	410.126	C\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022ab)
1,1,1,2,2,5,5,6,6,7,7,8,8,9,9,9-Hexadecafluoronon-3-ene	935477-04-6	-		$C_9H_2F_{16}$	414.089	FC(F)(F)C(F)(F)C=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022ac)

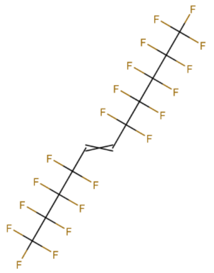
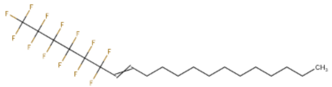
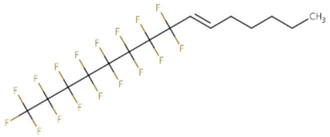
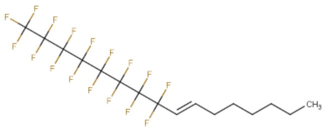
1,1,1,4,4,5,5,6,6,7,7,8,8,9,9,9-Hexadecafluoronon-2-ene	935477-01-3	-		$C_9H_2F_{16}$	414.089	FC(F)(F)C=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022ad)
1,1,1,2,2,3,3,6,6,7,7,8,8,9,9,9-Hexadecafluoronon-4-ene	935477-07-9	-		$C_9H_2F_{16}$	414.089	FC(F)(F)C(F)(F)C(F)(F)C=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022ae)
1,1,1,2,2,3,3,4,4-Nonafluorooctadec-5-ene	160460-03-7	-		$C_{18}H_{27}F_9$	414.4	CCCCCCCCCCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022af)
6E)-8,8,9,9,10,10,11,11,12,12,13,13,13-Tridecafluorotridec-6-ene	350608-60-5	-		$C_{13}H_{13}F_{13}$	416.226	CCCCC\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022ag)

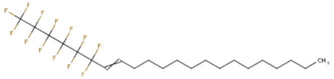
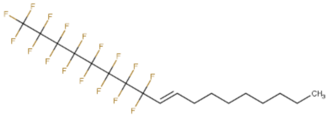
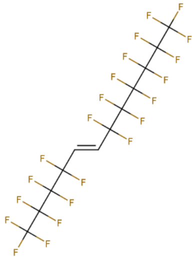
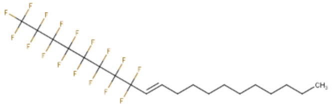
1,1,1,2,2,3,3,4,4,5,5,6,6-Tridecafluorotetradec-7-ene	120464-26-8	671-503-6		$C_{14}H_{15}F_{13}$	430.253	CCCCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022ah)
1,1,1,2,2,3,3,4,4,5,5,6,6-Tridecafluoropentadec-7-ene	1980786-99-9	-		$C_{15}H_{17}F_{13}$	444.28	CCCCCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022ai)
7,7,8,8,9,9,10,10,11,11,12,12,13,13,13-Pentadecafluorotridec-5-ene	52717-05-2	-		$C_{13}H_{11}F_{15}$	452.207	CCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022aj)
1,1,1,2,2,3,3,4,4,5,5,6,6-Tridecafluorohexadec-7-ene	120464-27-9	-		$C_{16}H_{19}F_{13}$	458.307	CCCCCCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022ak)
(7E)-1,1,1,2,2,3,3,4,4,5,5,6,6-	152128-75-1	-		$C_{16}H_{19}F_{13}$	458.307	CCCCCCCC\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022al)

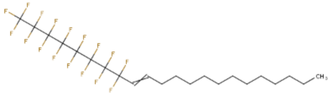
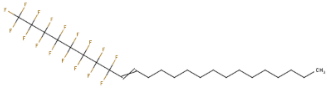
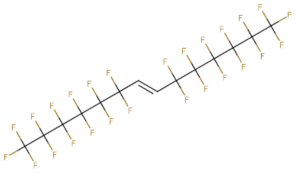
Tridecafluorohexadec-7-ene							
4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-Heptadecafluoroundec-2-ene	67103-04-2	-		$C_{11}H_5F_{17}$	460.134	CC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022am)
1,1,1,2,2,3,3,6,6,7,7,8,8,9,9,10,10,10-Octadecafluorodec-4-ene	935477-16-0	-		$C_{10}H_2F_{18}$	464.097	FC(F)(F)C(F)(F)C(F)(F)C=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022an)
1,1,1,2,2,5,5,6,6,7,7,8,8,9,9,10,10,10-Octadecafluorodec-3-ene	86563-87-3	-		$C_{10}H_2F_{18}$	464.097	FC(F)(F)C(F)(F)C=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022ao)

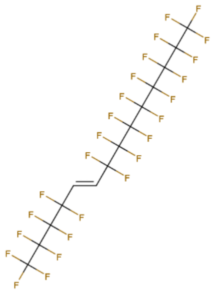
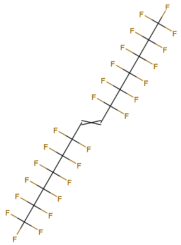
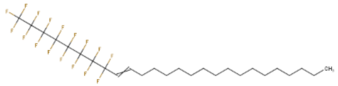
1,1,1,2,2,3,3,4,4,7,7,8,8,9,9,10,10,10-Octadecafluorodec-5-ene	84551-43-9	-		$C_{10}H_2F_{18}$	464.097	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022ap)
8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-Pentadecafluorotetradec-6-ene	38787-60-9	-		$C_{14}H_{13}F_{15}$	466.234	CCCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022aq)
(7E)-1,1,1,2,2,3,3,4,4,5,5,6,6-Tridecafluorooctadec-7-ene	125081-49-4	-		$C_{18}H_{23}F_{13}$	486.361	CCCCCCCCCC\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022ar)
1,1,1,2,2,3,3,4,4,5,5,6,6-Tridecafluorooctadec-7-ene	131851-05-3	-		$C_{18}H_{23}F_{13}$	486.361	CCCCCCCCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022as)

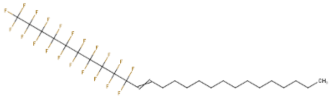
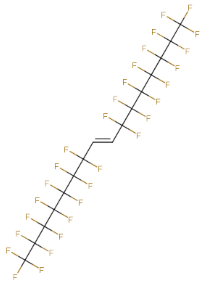
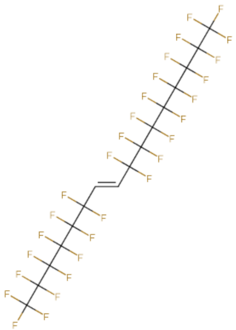
(5E)-7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-Heptadecafluorotetradec-5-ene	210491-04-6	-		$C_{14}H_{11}F_{17}$	502.215	CCCC\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022at)
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7-Pentadecafluoroheptadec-8-ene	52717-06-3	-		$C_{17}H_{19}F_{15}$	508.315	CCCCCCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022au)
1,1,1,2,2,3,3,6,6,7,7,8,8,9,9,10,10,11,11,11-Icosafluoroundec-4-ene	100603-63-2	-		$C_{11}H_2F_{20}$	514.105	FC(F)(F)C(F)(F)C(F)(F)C=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022av)

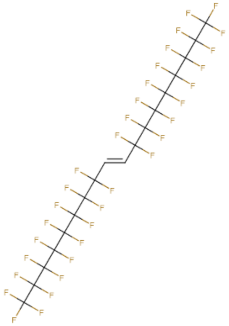
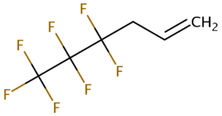
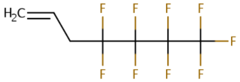
1,1,1,2,2,3,3,4,4,7,7,8,8,9,9,10,10,11,11,11-Icosafluoroundec-5-ene	100508-28-9	-		$C_{11}H_2F_{20}$	514.105	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022aw)
1,1,1,2,2,3,3,4,4,5,5,6,6-Tridecafluoroicos-7-ene	160460-04-8	-		$C_{20}H_{27}F_{13}$	514.415	CCCCCCCCCCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022ax)
(6E)-8,8,9,9,10,10,11,11,12,12,13,13,14,14,15,15,15-Heptadecafluoropentadec-6-ene	350608-65-0	-		$C_{15}H_{13}F_{17}$	516.242	CCCCC\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022ay)
(7E)-9,9,10,10,11,11,12,12,13,13,14,14,15,15,16,16,16-	84201-60-5	-		$C_{16}H_{15}F_{17}$	530.269	CCCCCC\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022az)

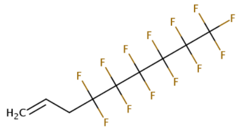
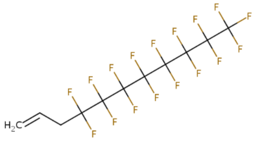
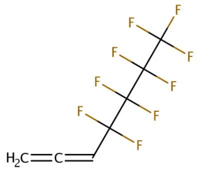
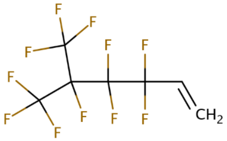
1,1,1,2,2,3,3,4,4,5,5,6,6-Tridecafluorodocos-7-ene	1244062-15-4	-		$C_{22}H_{31}F_{13}$	542.469	CCCCCCCCCCCCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022ba)
(9E)-1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-Heptadecafluorooctadec-9-ene	113999-61-4	-		$C_{18}H_{19}F_{17}$	558.323	CCCCCCCC\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bb)
(5E)-1,1,1,2,2,3,3,4,4,7,7,8,8,9,9,10,10,11,11,12,12,12-Docosafluorododec-5-ene	51249-66-2	-		$C_{12}H_2F_{22}$	564.113	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bc)
(9E)-1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-	124921-25-1	-		$C_{20}H_{23}F_{17}$	586.377	CCCCCCCCCC\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bd)

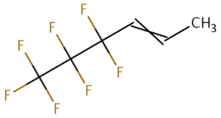
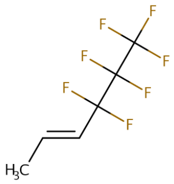
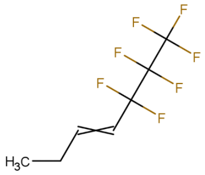
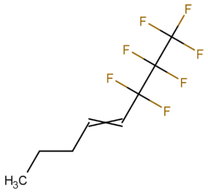
Heptadecafluoroicos-9-ene							
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-Heptadecafluorodocos-9-ene	118642-84-5	-		$C_{22}H_{27}F_{17}$	614.431	CCCCCCCCCCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022be)
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-Heptadecafluorotetracos-9-ene	1244062-16-5	-		$C_{24}H_{31}F_{17}$	642.485	CCCCCCCCCCCCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bf)
(7E)-1,1,1,2,2,3,3,4,4,5,5,6,6,9,9,10,10,11,11,12,12,13,13,14,14,14-Hexacosafluorotetradec-7-ene	51249-67-3	671-615-5		$C_{14}H_2F_{26}$	664.128	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bg)

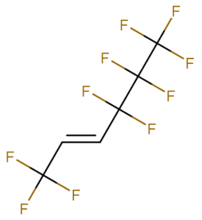
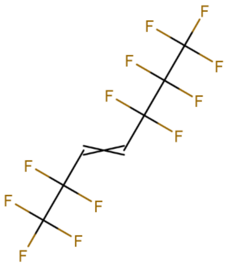
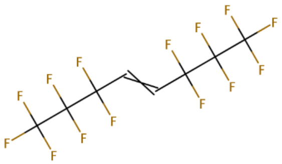
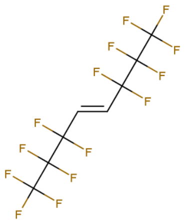
(5E)-1,1,1,2,2,3,3,4,4,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-Hexacosafluorotetradec-5-ene	51249-69-5	-		$C_{14}H_2F_{26}$	664.128	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bh)
1,1,1,2,2,3,3,4,4,5,5,6,6,9,9,10,10,11,11,12,12,13,13,14,14,14-Hexacosafluorotetradec-7-ene	56523-43-4	-		$C_{14}H_2F_{26}$	664.128	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bi)
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-Heptadecafluorohexacos-9-ene	907206-01-3	-		$C_{26}H_{35}F_{17}$	670.539	CCCCCCCCCCCCCCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bj)

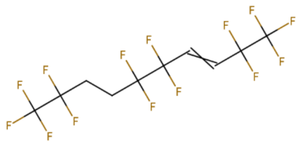
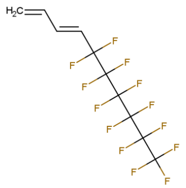
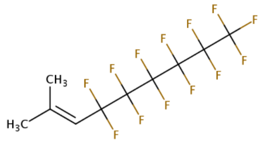
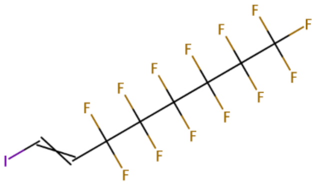
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-Henicosafluorohexacos-11-ene	1244062-18-7	-		$C_{26}H_{31}F_{21}$	742.5	CCCCCCCCCCCCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bk)
(8E)-1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,10,10,11,11,12,12,13,13,14,14,15,15,16,16,16-Triacontafluorohexadec-8-ene	35709-15-0	-		$C_{16}H_2F_{30}$	764.144	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bl)
(7E)-1,1,1,2,2,3,3,4,4,5,5,6,6,9,9,10,10,11,11,12,12,13,13,14,14,15,15,16,16,16-Triacontafluorohexadec-7-ene	51249-68-4	-		$C_{16}H_2F_{30}$	764.144	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bm)

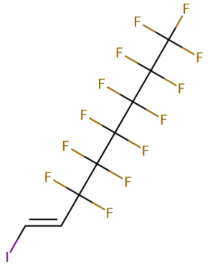
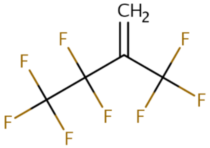
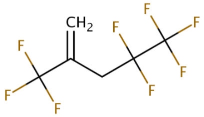
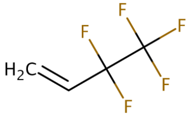
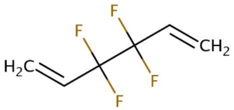
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-Pentacosafluorooctacos-13-ene	1151525-71-1	-		$C_{28}H_{31}F_{25}$	842.516	CCCCCCCCCCCCCCC=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bn)
(9E)-1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,11,11,12,12,13,13,14,14,15,15,16,16,17,17,18,18,18-Tetratriacontafluorooctadec-9-ene	51249-70-8	-		$C_{18}H_2F_{34}$	864.16	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)\C=C\C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bo)
4,4,5,5,6,6,6-Heptafluorohex-1-ene	2317-84-2	-		$C_6H_5F_7$	210.095	FC(F)(F)C(F)(F)C(F)(F)CC=C	US EPA (2022bp)
4,4,5,5,6,6,7,7,7-	129846-67-9	-		$C_7H_5F_9$	260.103	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)CC=C	US EPA (2022bq)

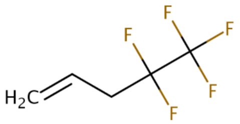
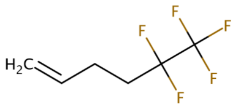
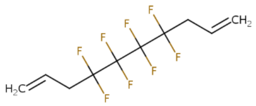
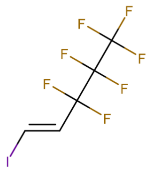
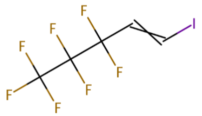
Nonafluorohept-1-ene							
4,4,5,5,6,6,7,7,8,8,9,9,9-Tridecafluoronon-1-ene	80793-18-6	-		$C_9H_5F_{13}$	360.118	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CC=C	US EPA (2022br)
4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-Heptadecafluoroundec-1-ene	61589-64-8	-		$C_{11}H_5F_{17}$	460.134	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CC=C	US EPA (2022bs)
4,4,5,5,6,6,7,7,7-Nonafluorohepta-1,2-diene	132673-98-4	-		$C_7H_3F_9$	258.087	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C=C=C	US EPA (2022bt)
3,3,4,4,5,6,6,6-Octafluoro-5-(trifluoromethyl)hex-1-ene	139060-76-7	-		$C_7H_3F_{11}$	296.083	FC(F)(F)C(F)(C(F)(F)F)C(F)(F)C(F)(F)C=C	US EPA (2022bu)

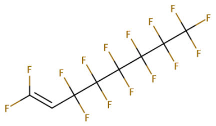
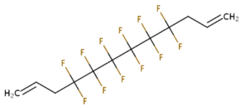
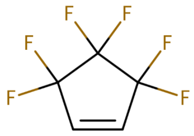
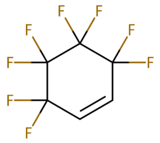
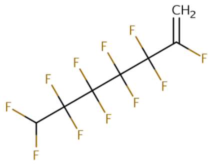
4,4,5,5,6,6,6-Heptafluorohex-2-ene	355-95-3	-		$C_6H_5F_7$	210.095	CC=CC(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bv)
(2E)-4,4,5,5,6,6,6-Heptafluorohex-2-ene	1081782-31-1	-		$C_6H_5F_7$	210.095	C\C=C\C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bw)
5,5,6,6,7,7,7-Heptafluorohept-3-ene	355-98-6	-		$C_7H_7F_7$	224.122	CCC=CC(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bx)
1,1,1,2,2,3,3-Heptafluorooct-4-ene	2707-72-4	-		$C_8H_9F_7$	238.149	CCCC=CC(F)(F)C(F)(F)C(F)(F)F	US EPA (2022by)

(2E)-1,1,1,4,4,5,5,6,6,6-Decafluorohex-2-ene	83227-62-7	-		$C_6H_2F_{10}$	264.066	FC(F)(F)\C=C\C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022bz)
1,1,1,2,2,5,5,6,6,7,7,7-Dodecafluorohept-3-ene	887111-61-7	-		$C_7H_2F_{12}$	314.074	FC(F)(F)C(F)(F)C=CC(F)(F)C(F)(F)C(F)(F)F	US EPA (2022ca)
1,1,1,2,2,3,3,6,6,7,7,8,8,8-Tetradecafluorooct-4-ene	3910-82-5	-		$C_8H_2F_{14}$	364.082	FC(F)(F)C(F)(F)C(F)(F)C=CC(F)(F)C(F)(F)C(F)(F)F	US EPA (2022cb)
(4E)-1,1,1,2,2,3,3,6,6,7,7,8,8,8-Tetradecafluorooct-4-ene	35709-14-9	-		$C_8H_2F_{14}$	364.082	FC(F)(F)C(F)(F)C(F)(F)\C=C\C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022cc)

1,1,1,2,2,5,5,6,6,9,9,10,10-Tetradecafluorodec-3-ene	35208-08-3	-		$C_{10}H_6F_{14}$	392.136	FC(F)(F)C(F)(F)CCC(F)(F)C(F)(F)C=CC(F)(F)C(F)(F)F	US EPA (2022cd)
(3E)-5,5,6,6,7,7,8,8,9,9,10,10-Tridecafluorodeca-1,3-diene	148626-04-4	-		$C_{10}H_5F_{13}$	372.129	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)\C=C\C=C	US EPA (2022ce)
4,4,5,5,6,6,7,7,8,8,9,9,9-Tridecafluoro-2-methylnon-2-ene	112343-55-2	-		$C_{10}H_7F_{13}$	374.145	CC(C)=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022cf)
3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluoro-1-iodooct-1-ene	150223-14-6	813-764-2		$C_8H_2F_{13}I$	471.988	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=CI	US EPA (2022cg)

(1E)-3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluoro-1-iodooct-1-ene	329698-26-2	-		$C_8H_2F_{13}I$	471.988	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)\C=C\I	US EPA (2022ch)
3,3,4,4,4-Pentafluoro-2-(trifluoromethyl)but-1-ene	189154-79-8	-		$C_5H_2F_8$	214.058	FC(F)(F)C(=C)C(F)(F)C(F)(F)F	US EPA (2022ci)
4,4,5,5,5-Pentafluoro-2-(trifluoromethyl)pent-1-ene	90277-98-8	-		$C_6H_4F_8$	228.085	FC(F)(F)C(=C)CC(F)(F)C(F)(F)F	US EPA (2022cj)
3,3,4,4,4-Pentafluorobut-1-ene	374-27-6	206-775-3		$C_4H_3F_5$	146.06	FC(F)(F)C(F)(F)C=C	US EPA (2022ck)
3,3,4,4-Tetrafluorohexa-1,5-diene	1763-21-9	217-178-2		$C_6H_6F_4$	154.108	FC(F)(C=C)C(F)(F)C=C	US EPA (2022cl)

4,4,5,5,5-Pentafluoropent-1-ene	135671-20-4	-		$C_5H_5F_5$	160.087	FC(F)(F)C(F)(F)CC=C	US EPA (2022cm)
5,5,6,6,6-Pentafluorohex-1-ene	106128-16-9	-		$C_6H_7F_5$	174.114	FC(F)(F)C(F)(F)CCC=C	US EPA (2022cn)
4,4,5,5,6,6,7,7-Octafluorodeca-1,9-diene	170804-07-6	-		$C_{10}H_{10}F_8$	282.177	FC(F)(CC=C)C(F)(F)C(F)(F)C(F)(F)CC=C	US EPA (2022co)
(1E)-3,3,4,4,5,5,5-Heptafluoro-1-iodopent-1-ene	157430-71-2	-		$C_5H_2F_7I$	321.964	FC(F)(F)C(F)(F)C(F)(F)\C=C\I	US EPA (2022cp)
3,3,4,4,5,5,5-Heptafluoro-1-iodopent-1-ene	376-97-6	-		$C_5H_2F_7I$	321.964	FC(F)(F)C(F)(F)C(F)(F)C=CI	US EPA (2022cq)

1,1,3,3,4,4,5,5,6,6,7,7,8,8,8-Pentadecafluorooct-1-enato	103712-63-6	-		C_8HF_{15}	382.072	FC(F)=CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	US EPA (2022cr)
4,4,5,5,6,6,7,7,8,8,9,9-Dodecafluorododeca-1,11-diene	170804-09-8	-		$C_{12}H_{10}F_{12}$	382.193	FC(F)(CC=C)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CC=C	US EPA (2022cs)
3,3,4,4,5,5-Hexafluorocyclopent-1-ene	1005-73-8	688-377-3		$C_5H_2F_6$	176.061	FC1(F)C=CC(F)(F)C1(F)F	US EPA (2022ct)
3,3,4,4,5,5,6,6-Octafluorocyclohex-1-ene	775-40-6	-		$C_6H_2F_8$	226.069	FC1(F)C=CC(F)(F)C(F)(F)C1(F)F	US EPA (2022cu)
2,3,3,4,4,5,5,6,6,7,7-Undecafluorohept-1-ene	94228-81-6	671-278-4		$C_7H_3F_{11}$	296.083	FC(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)=C	US EPA (2022cv)

Appendix C: QSAR models

Two main databases were used to source *in silico* data for this evaluation when required. These were the United States Environmental Protection Agency (US EPA) CompTox Dashboard (US EPA, 2022a) and the Royal Society of Chemistry (RSC) ChemSpider portal (RSC, 2022). Both integrate diverse types of relevant domain data through a cheminformatics platform, and are built upon a database of curated substance properties linked to chemical structures (Williams *et al*., 2017).

The QSAR models available from these two platforms are presented in Table C.1 (data from other open access models are available in the CompTox dashboard, but for the sake of brevity, these have not been used for the purposes of this evaluation).

Table C.1 QSAR model outline

Name	Brief description
ACD/Labs	Predicts physicochemical properties via the Percepta Platform[2].
EPISuite™ **Estimation Programs Interface Suite™ for Microsoft® Windows**	A Windows®-based suite of physical/chemical, environmental fate and ecotoxicity property estimation programs developed by the US EPA and Syracuse Research Corp. It uses a single input (typically a SMILES string) to run the following estimation programs: AOPWIN™, AEROWIN™, BCFBAF™, BioHCwin, BIOWIN™, ECOSAR™, HENRYWIN™, HYDROWIN™, KOAWIN™, KOCWIN™, KOWWIN™, LEV3EPI™, MPBPWIN™, STPWIN™, WATERNT™, WSKOWWIN™ and WVOLWIN™.
OPEn structure–activity/property Relationship App (OPERA)	Open source suite of QSAR models providing predictions and additional information including applicability domain and accuracy assessment, as described in Williams *et al*. (2017). All models were built on curated data and standardized chemical structures as described in Williams *et al*. (2016). All OPERA properties are predicted under ambient conditions of 760 mmHg (103 kPa) at 25 °C.

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[2] http://www.acdlabs.com/products/percepta/

Name	Brief description
T.E.S.T. Toxicity Estimation Software Tool	US EPA software application for estimating the toxicity of chemicals using QSAR methods. EPISuite™ is the model used to generate some physico-chemical data, although T.E.S.T. does not report K_{OW} values and uses a different database for surface tension. (US EPA, 2016).

EPISuite™

Table C.2 summarises the PFCs identified in the training/validation sets for EPISuite™. Applicability domain (US EPA, 2022cx).

Table C.2 EPISuite™ PFCs included in training and validation sets

EPISuite model	Training set	Validation set
MPBPVP v 1.42	tetrafluoromethane hexafluoroethane tetrafluoroethylene octafluoropropane hexafluoropropene decafluorobutane perfluorocyclobutane perfluoro-n-hexane perfluorocyclohexane perfluoroheptane perfluoromethylcyclohexane	not available
WSKOWWIN v 1.41	none identified	octafluoropropane octafluorocyclobutane
Water solubility estimate from fragments (WATERNT v 1.01 est)	trifluoromethane	tetrafluoromethane hexafluoroethane octafluoropropane perfluorocyclobutane tetrafluoroethylene
KOAWIN v 1.1	Uses KOWWIN and HENRYWIN databases	
KOCWIN v 1.66	none identified	none identified
KOWWIN v 1.67	tetrafluoromethane hexafluoroethane	perfluorocyclohexane
HENRYWIN v 3.1	tetrafluoromethane hexafluoroethane tetrafluoroethene	octafluoropropane perfluorocyclobutane

Open Structure-activity/property Relationship App (OPERA)

OPERA is a free and open-source/open-data suite of QSAR models providing predictions for physicochemical properties, environmental fate parameters, and toxicity endpoints.

Applicability domain (AD) (Williams *et al.,* 2017):

- If a chemical is considered outside the global AD and has a low local AD index (< 0.4), the prediction can be unreliable.
- If a chemical is considered outside the global AD but the local AD index is average (0.4–0.6), the query chemical is on the boundary of the training set but has quite similar neighbours (average reliability). If the local AD index is high (> 0.6), the prediction can be trusted.
- If a chemical is considered inside the global AD but the local AD index is average (0.4–0.6), the query chemical falls in a “gap” of the chemical space of the model but still falls within the boundaries of the training set and is surrounded with training chemicals. The prediction therefore should be considered with caution.
- If a chemical is considered inside the global AD and has a high local AD index (> 0.6), the prediction can be considered reliable.

T.E.S.T. (Toxicity Estimation Software Tool)

Data sets used in T.E.S.T. (US EPA, 2016) for parameters reported at 25 °C:

- Surface tension: Dataset for 1 416 chemicals obtained from the data compilation of Jasper 1972;
- Water solubility: Dataset of 5 020 chemicals was compiled from the database in EPI Suite^{TM}. Chemicals with water solubilities exceeding 1,000,000 mg/L were omitted from the overall dataset;
- Vapour pressure: Dataset of 2 511 chemicals was compiled from the database in EPI Suite^{TM}.

T.E.S.T. displays structures for substances from the test and training sets that are closest to the substance where a predicted value is required. A comparison between the experimental and predicted value for the substances in the test and training sets provides a similarity coefficient. If the predicted values match the experimental values for similar chemicals in the test and training set (and the similar chemicals were predicted well), there is greater confidence in the predicted value for the substance under evaluation

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