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Environmental risk evaluation report: Annex B: Read-across of environmental data between aryl phosphates

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Steve Killeen

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Head of Science

Introduction

This annex considers the read-across of data between the triaryl and aryl/alkyl phosphates assessed in this series, to fill in data gaps in the key physico-chemical properties and ecotoxicity data required for environmental risk assessment. The data available for the individual substances are discussed in detail in the main reports.

The approach taken here is to relate the measured physico-chemical properties and ecotoxicity data for the various substances to a parameter that can be easily predicted for all substances considered. In this case, the Syracuse Research Corporation EPI software estimates of log K_{ow} and vapour pressure are used as parameters that can be easily calculated from the chemical structure of the substance. In this way, any missing data values for a given property can be readily predicted from the estimate obtained from the EPI software.

In the analysis, the EPI estimate of log K_{ow} is used to effectively normalise the available measured data on solubility, log K_{ow} and ecotoxicity. There is some logic behind using the estimated log K_{ow} for this process, as many quantitative structure activity relationships relate parameters such as solubility and ecotoxicity to the log K_{ow}. For the analysis of vapour pressure data, the EPI estimate for the vapour pressure is used to effect the normalisation.

Table B 1 outlines the measured data available for the various endpoints considered, along with respective estimates for log K_{ow} and vapour pressure obtained from the chemical structure using the EPI software.

Figures B1 to B6 show the plots of the various measured data against EPI-estimated log K_{ow} or vapour pressure. The regression equations obtained from these plots are summarised below.

The use of predictive data needs to be considered with caution. A complicating factor is that most of the commercial substances are complex mixtures, and it is apparent that some mammalian toxicological effects may be influenced by isomerism. Nevertheless, they are all assumed to behave as single substances for the purposes of this review (since this is currently the only practical approach). In addition, many of the correlations obtained are poor and the validity of the approach taken could be questioned on this basis. However, there are a number of gaps in the data available for some aryl phosphate esters and, in the absence of actual test data, the only alternative to the approach taken would be to use the EPI estimates (or other estimates which tend to be based on K_{ow} for solubility, bioconcentration factor (BCF) and toxicity using the estimation methods given in the Technical Guidance Document or TGD) for the various endpoints. As discussed in the individual risk evaluation reports (and is apparent from the plots in this annex), for substances where data are available, the estimated data are often in relatively poor agreement with the measured value, and so using the estimated data alone to fill data gaps would probably lead to substantial errors. Therefore, despite the limitations and uncertainties in the regressions obtained, the approach taken in this annex (essentially normalising the EPI estimates of log K_{ow} to the available measured data) should give more reliable estimates for the data gaps than could be obtained using the EPI or TGD estimates alone.

Where the data derived here are important to the conclusion of the risk assessment (for example, toxicity data), uncertainties in the use of the data are discussed in the main risk evaluation reports and recommendations for reducing this uncertainty are given.

Table B 1 Data used for estimating missing values.

Phosphate ester	Property								
	Measured vapour pressure at 20°C (Pa)	Measured water solubility at room temperature (mg/l)	Measured Log K_{ow}	Measured BCF (l/kg)	Long-term NOEC for aquatic organisms (mg/l)			EPI Estimates	
					Fish	Invertebrates	Algae	Vapour pressure at 25°C (Pa)	Log K_{ow}
Triphenyl phosphate	1.2×10^{-3}	1.9	4.63	420	0.037		0.1	2.8×10^{-5}	4.70
Trixylenyl phosphate	[4.7×10^{-4}][a]	0.89	5.63	1,300-1,900				2.7×10^{-6}	7.98
Tricresyl phosphate	3.5×10^{-5}	0.36	5.11	800	0.00032	0.1	0.32	3.4×10^{-6}	6.34
Cresyl diphenyl phosphate	3.3×10^{-5}	2.6	4.51	200				1.4×10^{-5}	5.24
Tris(isopropylphenyl) phosphate	2.3×10^{-6}				0.024[b]	0.006[b]		2.7×10^{-6}	9.07
Isopropylphenyl diphenyl phosphate	9.5×10^{-6}	2.2	5.30	[7,266][a]	0.024[b]	0.006[b]		5.3×10^{-6}	6.16
Tertbutylphenyl diphenyl phosphate	7.8×10^{-5}	0.04-3.2	5.12	778	0.093	0.010		3.5×10^{-6}	6.61
2-Ethylhexyl diphenyl phosphate	3.4×10^{-4}	0.38-1.9[c]	5.73	934	0.021	0.018		2.5×10^{-5}	6.30
Isodecyl diphenyl phosphate	[3.8][a]	0.03-0.75[c]	5.44	335	0.057	0.004		6.3×10^{-6}	7.28
Tetraphenyl resorcinol diphosphate		0.69				>0.064		2.7×10^{-6}	7.41

Notes: a) These values are uncertain (see main risk assessment reports) and have not been included in the estimation analysis.
b) Assumes these two products have similar toxicity.
c) Revised solubilities used in the individual risk assessment reports, the values here are used in the estimation analysis.

Physico-chemical properties

Vapour pressure

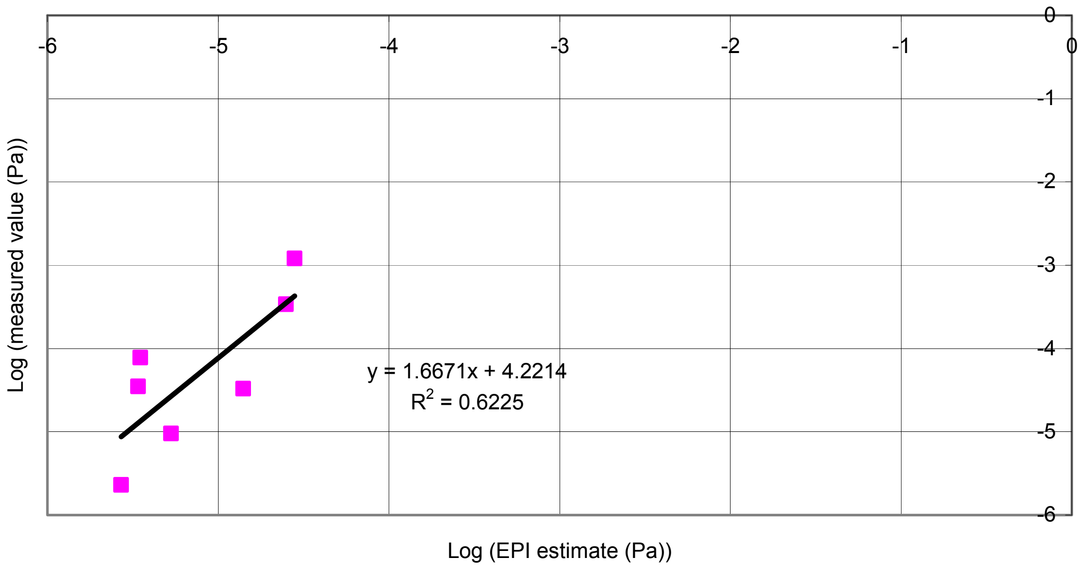
The plot (Figure B1) was constructed omitting the data point for isodecyl diphenyl phosphate (which appears to be out of line with the other available data). A reasonable correlation was obtained between the log (measured vapour pressure at 20°C (Pa)) and the log (EPI-estimated vapour pressure at 25°C (Pa)). The following regression equation was obtained:

log (measured vapour pressure at 20°C (Pa) = 1.6671 × log (EPI estimate (Pa)) + 4.2214

Using this equation, the vapour pressures at 20°C can be estimated for the data gaps as follows:

Tris(isopropylphenyl) phosphate	8.5×10^{-5} Pa
Isopropylphenyl diphenyl phosphate	1.1×10^{-4} Pa
Isodecyl diphenyl phosphate	3.6×10^{-5} Pa
Tetraphenyl resorcinol disphosphate	8.7×10^{-6} Pa
Trixylenyl phosphate	8.7×10^{-6} Pa

Figure B1: Plot of log (measured vapour pressure (Pa) against log (EPI estimated vapour pressure (Pa)).



Water solubility

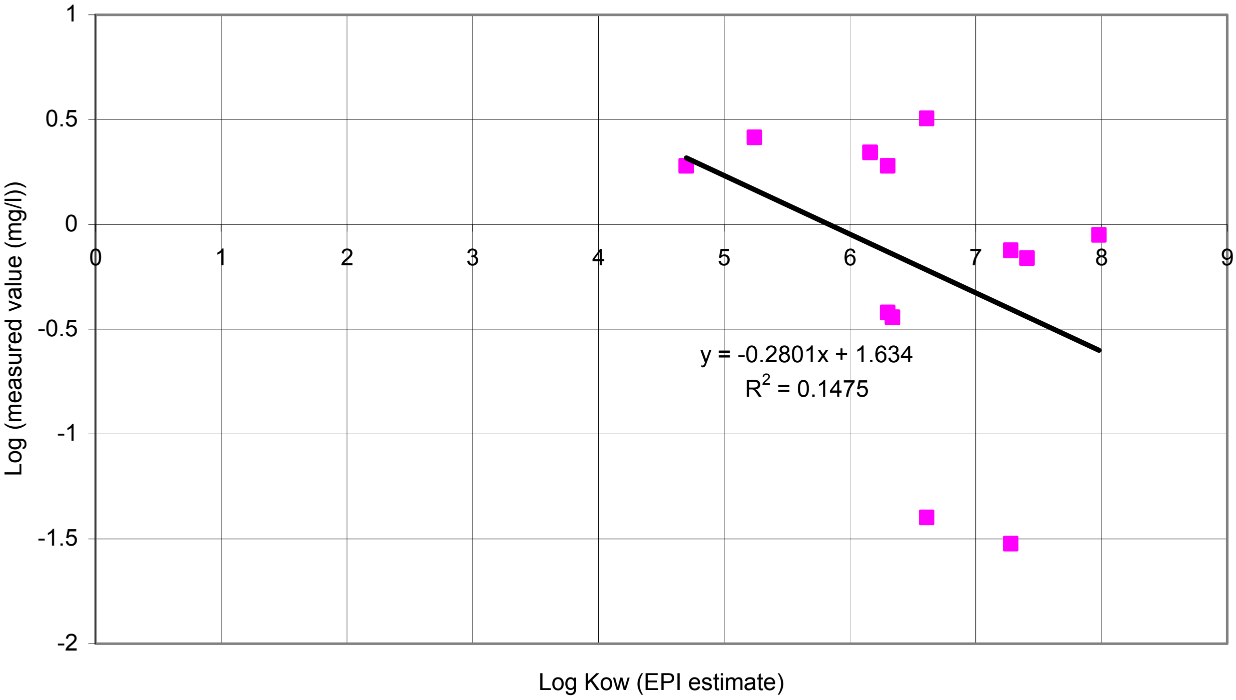
A poor correlation (Figure B2) was obtained between the log (measured water solubility (mg/l)) and the log (EPI-estimated K_{ow}). The following regression equation was obtained:

$$\log (\text{measured water solubility}) = -0.2801 \times \log (\text{EPI-estimated } K_{ow}) + 1.634$$

Using this equation, the water solubility at room temperature can be estimated for the data gaps as follows:

Tris(isopropylphenyl) phosphate 0.12 mg/l

Figure B2: Plot of log (measured solubility (mg/l) at 20oC) against log Kow (EPI estimate).



Log K_{ow}

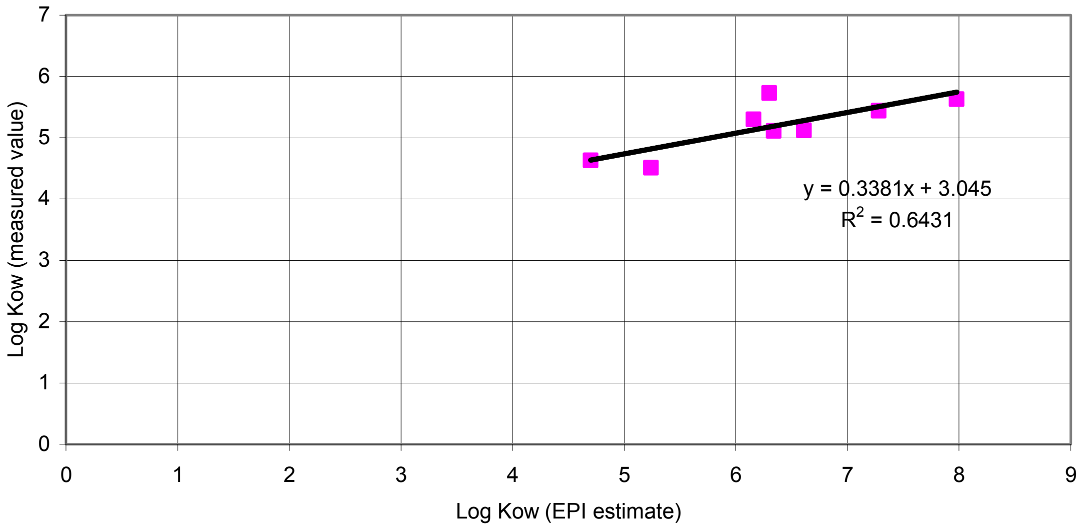
A reasonable correlation (Figure B3) was obtained between the log (measured K_{ow}) and the log (EPI-estimated K_{ow}). The following regression equation was obtained:

$$\log (\text{measured } K_{ow}) = 0.3381 (\text{EPI-estimated } K_{ow}) + 3.045$$

Using this equation, the log K_{ow} can be estimated for the data gaps as follows:

Tetraphenyl resorcinol diphosphate	5.5
Tris(isopropylphenyl) phosphate	6.1

Figure B3: Plot of log Kow (measured value) against log Kow (EPI estimate).



Environmental fate and behaviour

Bioconcentration factor, BCF

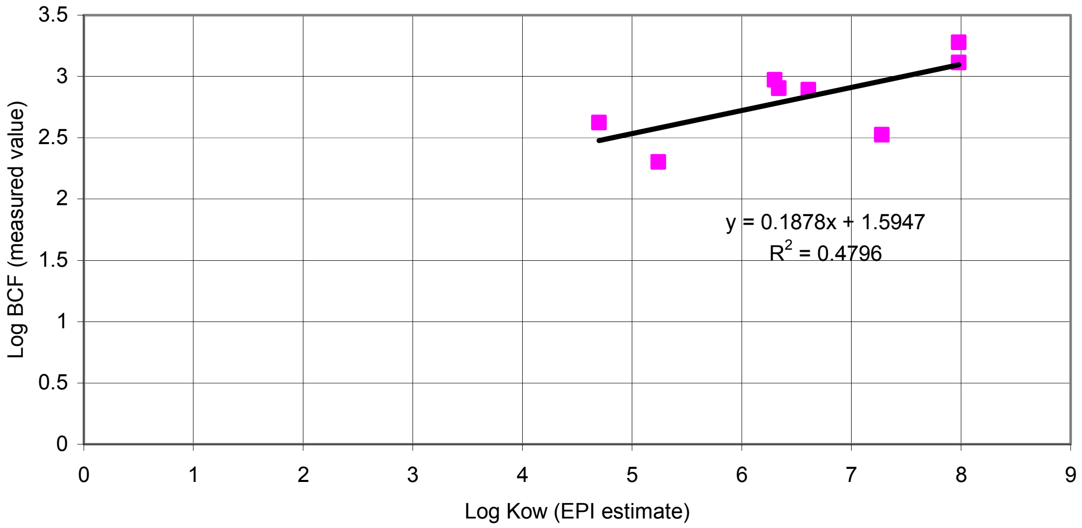
A reasonable correlation (Figure B4) was obtained between the log (measured BCF) and the log (EPI-estimated K_{ow}) when the data for isopropylphenyl diphenyl phosphate is omitted (this data point is considered an outlier). The following regression equation was obtained:

$$\log(\text{measured BCF}) = 0.1878 \times \log(\text{EPI-estimated } K_{ow}) + 1.5947$$

Using this equation, the BCF can be estimated for the data gaps as follows:

Tetraphenyl resorcinol diphosphate	BCF = 969 l/kg
Tris(isopropylphenyl) phosphate	BCF = 1,986 l/kg
Isopropylphenyl diphenyl phosphate	BCF = 564 l/kg
Tertbutylphenyl diphenyl phosphate	BCF = 686 l/kg
Trixylenyl phosphate	BCF = 1,240 l/kg

Figure B4: Plot of log BCF (measured value) against log Kow (EPI estimate).



Ecotoxicity

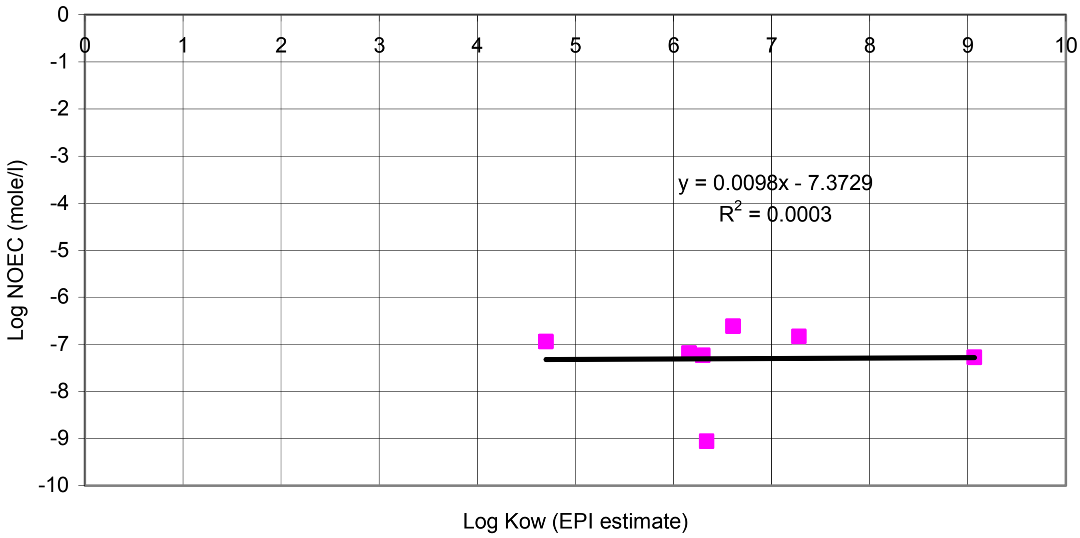
Long-term toxicity to fish

A plot of the log (no observed effect concentration (NOEC) for fish (mole/l)) against the log (EPI-estimated K_{ow}) is shown as Figure B5. The analysis combines the data from long-term fish growth/mortality studies and fish early life-stage studies. No clear trend with EPI-estimated K_{ow} was seen. This indicates that as a first approximation, the toxicities of the various trialkyl and trialkyl/aryl phosphates to fish are similar when expressed on a mol/l basis. The one exception appears to be tricresyl phosphate that has a fish NOEC considerably lower than the other phosphate esters considered here.

Assuming that all of the substances considered have a fish NOEC equivalent to around 4.2×10^{-8} mol/l (equivalent to the intercept of -7.3729 on Figure B5), the NOECs for the following substances for which data are not available can be estimated using the equation given in Figure B5:

Tetraphenyl resorcinol diphosphate	NOEC ~ 0.024 mg/l
Cresyl diphenyl phosphate	NOEC ~ 0.014 mg/l
Trixylenyl phosphate	NOEC ~ 0.017 mg/l
Tertbutylphenyl diphenyl phosphate	NOEC ~ 0.016 mg/l
Isodecyl diphenyl phosphate	NOEC ~ 0.016 mg/l
Isopropylphenyl diphenyl phosphate	NOEC ~ 0.015 mg/l
Tris(isopropylphenyl) phosphate	NOEC ~ 0.019 mg/l

Figure B5: Plot of log (NOEC (mole/l)) against log Kow (EPI estimate) for long-term fish toxicity.



One of the NOEC values (for tricresyl phosphate with *Gasterosteus aculeatus*) appears to be much lower than the other data. This substance/data point could therefore be considered an outlier. However, this value was obtained with a species for which data are lacking for the other aryl phosphate esters, and the other available long-term toxicity data for tricresyl phosphate with other fish species are not out of line with the data on other aryl phosphates. Therefore, it is not clear whether a) *Gasterosteus aculeatus* is particularly sensitive to aryl phosphates in general or b) if tricresyl phosphate shows a specific mode of action to *Gasterosteus aculeatus*. The above regression plot and equation was derived from the dataset including the tricresyl phosphate NOEC for *Gasterosteus aculeatus.* If this value is excluded, the regression equation becomes:

$$\log \text{NOEC (mol/l)} = -0.0485 \times \log (\text{EPI-estimated } K_{ow}) - 6.6916 \; (R^2 = 0.0713)$$

Long-term toxicity to invertebrates

A poor correlation was obtained between the log (NOEC for invertebrates (mol/l)) and the log (EPI-estimated K_{ow}). The following regression equation was obtained:

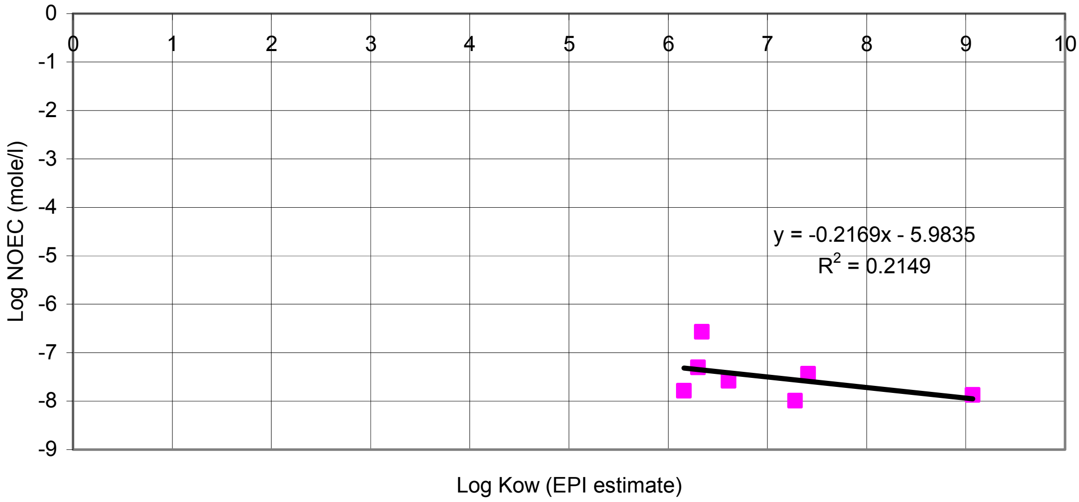
$$\log (\text{measured BCF}) = -0.2279 \times \log (\text{EPI-estimated } K_{ow}) - 5.9317$$

Using this equation, the log K_{ow} can be estimated for the data gaps as follows:

Tetraphenyl resorcinol diphosphate[1]	NOEC = 0.014 mg/l
Cresyl diphenyl phosphate	NOEC = 0.025 mg/l
Trixylenyl phosphate	NOEC = 0.007 mg/l
Triphenyl phosphate	NOEC = 0.032 mg/l

[1] The available long-term invertebrate data for tetraphenyl resorcinol diphosphate show that the actual NOEC is 0.021 mg/l; as there is some uncertainty in this value (undissolved test substance may have been present), it was not included in the analysis in Figure B6.

Figure B6: Plot of log NOEC (mole/l) against log Kow (EPI estimate) for long-term toxicity to invertebrates.



Long-term toxicity to algae

There are insufficient data to generate a regression equation for the algal NOEC. However, the available data indicate that algae appear to be much less sensitive than fish and invertebrates to triaryl and trialkyl/aryl phosphates and so an assessment based on the long-term fish and invertebrate data should also be protective for algae.

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