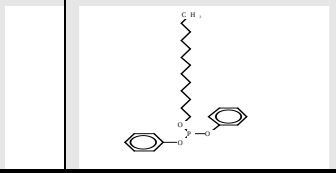
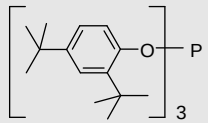
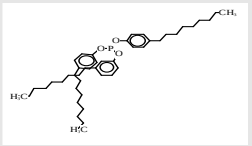
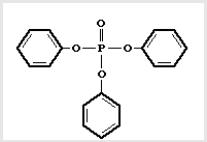
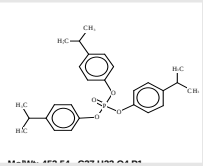
ANNEX 2: INFORMATION ON ANALOGOUS SUBSTANCES OF TNPP FOR READ-ACROSS

Table 1 : summary of key properties of TNPP and analogues

Substance name	Diphenyl monotridecyl phosphite	Tris(2,4-di-tert-butylphenyl)phosphite	Tri(nonylphenyl)phosphite / TNPP	Triphenyl phosphate / TPP	Tris(isopropylphenyl) phospate
Source	TNO, 2007	SIAR sponsored by UK and accepted at SIAM 18	This assessment	SIAR sponsored by Germany and accepted at SIAM 15	TNO, 2007
CAS	60628-17-3	31570-04-4	26523-78-4	115-86-6	26967-76-0
Molecular weight	416.55	646	689	326.29	452.54
Molecular formula	$C_{25}H_{37}O_3P_1$	$C_{42}H_{63}O_3P$	$C_{45}H_{69}O_3P$	$C_{18}H_{15}O_4P$	$C_{27}H_{33}O_4P_1$
Structural formula					
Physical state	-	Solid	Liquid	Solid	-
Melting point (°C)	-	180-186[1]	6 ± 3	48-50	-
Boiling point (°C)	-	Decomposes at >350	322°C (decomposition)	245	-
Density	-	1.03 g/cm^2 (20°C)	0.98 g.cm^{-3}	1.205	-
Vapour pressure (Pa)	2.03x10^{-9} (calc.)	1.3E-8 (20°C)[2]	0.058 at 25°C (extrapolated using measurements with the isoteniscope method) 5x10^{-12} (QSAR)	8.35E-4 (measured)	2.06x10^{-8} (calc.)
Water solubility (mg/L)	6.1x10^{-6} (cal.)	<0.005 (20°C)	~0.05 (LOQ) 3x10^{-16} (QSAR)	1.9 in distilled water	2.6x10^{-5} (calc.)

[1] All entries were assigned a reliability rating of 4, but the 'weight of evidence' approach has been taken to determine that the temperature range is reliable.

[2] This value is a measured value (assigned a reliability rating of 4). The value is supported by a similar calculated value (with a recognised method).

Substance name	Diphenyl monotridecyl phosphite	Tris(2,4-di-tert-butylphenyl)phosphite	Tri(nonylphenyl)phosphite / TNPP	Triphenyl phosphate / TPP	Tris(isopropylphenyl) phospate
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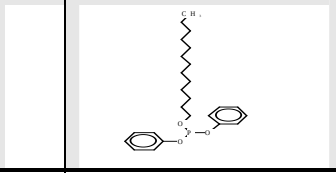
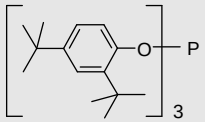
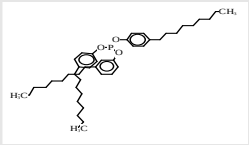
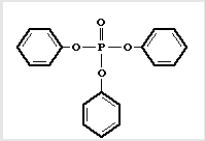
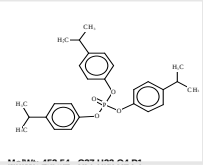
Structural formula					
Aryl Carbon	12	18	18	18	18
Alkyl Carbon	13	24	27	0	9
Partition coefficient n-octanol/water (log value)	10.07 (calculated)	18.8 (calculated)	20 (QSAR)	4.6 (measured) 4.7 (calculated)	9.07 (calc.)
BCF (L/kg)	<113 (measured)	3.6-109 (measured[3])	3.162 (QSAR)	110-114 (measured) 113 (calculated)	6.9-43 (measured) 15.7 (calc.)
Henry's law constant ($Pa.m^3.mol^{-1}$)	-	7.2E-03	66.1 (QSAR) >799 (TGD equation)	-	-

[3] BCF studies have not been validated due to the lack of information on the experimental conditions

Use of read-across to estimate log Kow and bioaccumulation potential of Tri(nonylphenyl)phosphite (TNPP)

Read-across from other alkyl triaryl phosphite compounds

Kow

Measured log KOW data for molecular structures of similar molecular weight and size to TNPP were lacking in the literature. Data was only found for lower molecular weight phosphites (TNO, 2007).

Bioaccumulation

Two experimental BCF-values were found for phosphites. For diphenyl monotridecyl phosphite (CAS No. 60628-17-3, 12 aromatic and 13 aliphatic carbons) the 42 day BCF for carp (Cyprinus caprio) was less than 113, while the BCF-value calculated with EPIWIN was estimated to be even lower at 4.1.

For tris(2,4-di-tert-butylphenyl) phosphite (CAS No. 31570-04-4, 18 aromatic and 24 aliphatic carbons) which is symmetric and considered to be similar to TNPP (28 aromatic and 27 aliphatic carbons) the measured BCF-value was 4.66 after 60 days of exposure in carp (IUCLID). The BCF value calculated with EPIWIN was in the same order of magnitude at 3.2 (TNO, 2007).

Read-across from alkyl triaryl phosphate compounds

Kow

The log KOW values calculated with EPIWIN, were in general, in good agreement with the available experimentally derived log KOW values. With some exceptions, like for isodecyl diphenyl phosphate (CAS No. 29761-21-5) the calculated log KOW from EPIWIN (7.28) was much higher than the experimentally derived log KOW value of 5.44 (Saeger et al. 1979) as was also observed for tri-m-cresyl phosphate (CAS No. 563-04-2; 6.43 vs 5.11) and tert-butylphenyl diphenyl phosphate (CAS No. 056803-37-3; 6.61 vs. 5.12), indicating that the calculated values are generally overestimated for this type of compounds (TNO, 2007).

Bioaccumulation

The experimentally derived BCF-values for (halo)alkyl phosphates are all low and do not exceed 60 L/kg. The experimental BCF-values do not always followed the predicted BCF-values (0.43-67 L/kg), but the difference never exceeded a factor of ~50. BCF values did not differ much between different fish species tested, although for Carassius auratus (goldfish) the BCF was often lower than the BCF for Oryzias latipes (medaka), but BCF-values of Cyprinus carpio (fathead minnow) often overlapped the BCF-values of C. auratus and O. latipes (TNO, 2007).

Details of information available for Tris(2,4-di-tert-butylphenyl)phosphite

Source: UNEP, 2005

Bioaccumulation

Exposure of carps to radiolabelled tris(2,4-di-tert-butylphenyl)phosphite during 60 days gave bioaccumulation factors below 100. No plateau phase was reached during the study period. The substance was tested at levels above the water solubility (0.1 and 1 ppm) and a dispersant was added to the medium (ref. 33). In addition unlabelled tris(2,4-di-tert-butylphenyl)phosphite was tested in carps during 60 days (again with the use of a dispersant). The result of this test was an overall quantitative bioconcentration factor of 3.6 (ref. 33). In a test with gold fish (duration 3 days), 16.6% of the radiolabel was found in water, while 6.3% accumulated in fish. A BCF (3 day) of 109 was recorded. It is not possible to assign a quality score to these tests due to a lack of information on the methodology used (ref.30).

Conclusion: Tris(2,4-di-tert-butylphenyl)phosphite has a high molecular weight (647 g/mol), has extremely low water solubility (<0.005 mg/L) and is highly sorptive. The high log Kow for the substance would indicate a potential for bioaccumulation, although it is recognised that a true measure of the bioconcentration remains uncertain. For substances with high log Kow, it is known that QSAR determinations of BCF (bioconcentration factor) may not accurately represent true bioaccumulation potential. The experimental evidence suggests that the potential for bioconcentration is low, although the quality of this test could not be assigned. The quality of the tests was also limited by the use of dispersants. Since the bioavailability of this dispersed material is difficult to determine, there is uncertainty as to the true level of the BCF.

Details of information available for the substance Triphenyl phosphate

Source: UNEP, 2003

Bioaccumulation of triphenyl phosphate:

In a continuous flow through test (0.01 mg/l TPP) with Oryzias latipes and an exposure period of 18 days a bioconcentration factor (BCF) of 144 (whole body) was determined. As the uptake of triphenyl phosphate in fish increased gradually till day 18 of exposure, it is not clear whether equilibrium was reached. The biological half-life in fish tissue was reported to be 1.2 h [Sasaki et al. 1982]. In a static test with Carassius auratus a BCF of 110 (whole body) was determined after 72 h of exposure to 0.25 mg/l TPP [Sasaki et al. 1981]. Also for this study it is unclear whether equilibrium was reached. The experimentally obtained BCF value is supported by the SRC-BCFWIN v2.14 (2000) [Bayer AG, 2002c] estimation with a correction factor for phosphate ester chemicals. The calculated BCF value for fish is 113.3.On the basis of the experimental results a moderate bioaccumulation potential for triphenyl phosphate can be assumed.

Measured bioconcentration factors in fish are in the range of 110 to 144, indicating a moderate bioaccumulation potential. BCF calculation with generic estimation equations should include a correction factor for phosphate ester chemicals. As the substance was found in dolphins an accumulation via the food chain has to be assumed.

References

1. TNO (2007). An assessment of the bioaccumulative potential of tris(nonylphenyl)phosphite (TNPP) in aquatic biota. Zeist, 31st July 2007, TNO: 36.
2. UNEP (2003). OECD SIDS Initial Assessment Report for Triphenylphosphate (CAS 115-86-6) sponsored by Germany and adopted at SIAM 15 (October 2002).
3. UNEP (2005). OECD SIDS Initial Assessment Report for Tris(2,4-di-tert-butylphenyl)phosphite (CAS 31570-04-4) sponsored by United Kingdom and adopted at SIAM 18 (April 2004).