

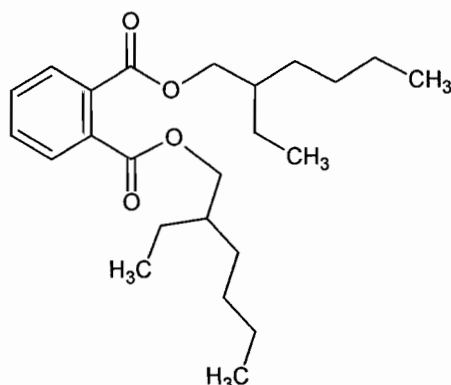
1

GENERAL SUBSTANCE INFORMATION

1.1

IDENTIFICATION OF THE SUBSTANCE

CAS Number: 117-81-7
EINECS Number: 204-211-0
IUPAC Name: Bis(2-ethylhexyl) phthalate
Molecular formula: $C_{24}H_{38}O_4$
Structural formula:



Molecular weight: 390.6
Synonyms: 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester
Bis(2-ethylhexyl) 1,2-benzenedicarboxylate
Bis(2-ethylhexyl) o-phthalate
Bis(2-ethylhexyl) phthalate
DEHP
Di(2-ethylhexyl) phthalate
Dioctyl phthalate
DOP (pseudo-synonym, incl. also other isomeric forms of the alcohol part)
Phthalic acid dioctyl ester
Phthalic acid, bis(2-ethylhexyl) ester
Trade names: FLEXOL Plasticizer DOP Union carbide
Essochem DOP ESSO
Palatinol AH BASF AG
Palatinol AH-L (med.) 99.5% BASF AG
Genomoll 100 99.7% Hoechst AG
Vestinol AH 99.5% Hüls AG 1994a

1.2

PURITY/IMPURITIES, ADDITIVES

Purity/impurity

Only few data about the purity are available. This indicates a high purity level (99.7%). The impurities found are mainly other phthalates (Hüls AG 1995g).

Additives

“Bisphenol A”; 4,4'-isopropylidenediphenol (synonyms e.g.: diphenylolpropane; 2,2-bis(p-hydroxyphenyl)-propane). CAS No. 80-05-7. Some customers request this additive in the range of 0.025 to 0.5% (ECPI 1998a).

1.3 PHYSICO-CHEMICAL PROPERTIESPhysical state

DEHP is a colourless oily liquid at normal temperature.

Melting-point

-50°C (Sorbe 1984, in Rippen 2005), -55°C (pour point, BUA 1986; CRC 1995)

Boiling-point

Approximately 230°C at 5 mm Hg (BASF1994b; Clayton 1981, in HSDB 2005)

385°C at 1013 hPa (Verscheuren 1983 and Sorbe 1984 in Rippen 2005)

Density

0.984 g/cm³ at 20°C (OECD 1979, in Rippen 2005)

0.986 g/cm³ at 20°C (IARC 1982, in HSDB 2005)

0.980-0.985 g/ml (Furtmann 1996)

Vapour pressure

A large range of values on the vapour pressure is available in the literature (0.00000004 - 0.0014 Pa, Staple et al. 1997b). However, recent studies have shown that many of these values probably are overestimations due to interference from impurities (Rippen 1992). In a newly made measurement with 99.5% pure DEHP, the vapour pressure was estimated to 0.000034 Pa at 20°C (See Table below) (Hüls AG 1997). This value is used for assessing the environmental fate.

°C	Pa	Comment
10	0.000010*	
15	0.000023	
20	0.000034*	used in EUSES / fugacity
30	0.00013*	
40	0.00047*	
50	0.0016*	
60	0.0057	

70	0.011	max. indoor car (BUA 1986)
80	0.039	
90	0.10	
100	0.29	
110	0.76	
120	1.9	
140	4.5*	
160	2.4*	injection moulding, PVC
180	80*	
203	287	
210	389	
216	511	

* Extrapolated values

Water solubility

A large range of values on the water solubility is available in the literature (0.003-1.3 mg/l at 20-25°C) (see **Table 1.1**). A probable explanation of this is that DEHP easily forms more or less colloidal dispersions in water, which increase the amount DEHP in the water phase (Lundberg and Nilsson 1994). The colloidal formation might be of relevance in understanding laboratory studies in aquatic media. A colloidal water solubility of about 0.34 mg/l (ECETOC 1985) is assumed in this assessment. However, the non-colloidal solubility is more relevant to the fugitive long-term distribution in the environment. Staples et al. (1997) reviewed present studies on water solubility and compared these with different calculated values. Based on these they suggested a non-colloidal solubility of 0.003 mg/l (the temperature for this solubility was not mentioned). An alternative method to get round the colloidal disturbance was developed by Thomsen et al. 2001. By measuring the surface tension the solubility in water was estimated to be about 0.017 mg/l at 22°C. The authors suggest that the deviation from earlier estimations based on slow stirring technique may depend on high affinity for adsorption at interfaces of laboratory equipment. This then may reduce the accuracy in the recovery of DEHP. Available studies clearly show considerable difficulties in estimating relevant water solubility. In a bioaccumulation study on fish (Mehrlé and Mayer, 1976; Mayer 1976) made at different concentration between 1.9 to 62 µg/l a sharp reduction in the BCF was observed between 4.6 and 8.1 µg/l (see **Table 3.44**). A probable explanation is that at test concentrations over 4.6 µg/l DEHP is dosed over the non-colloidal water solubility (assuming a lower bioavailability for colloidal/precipitated DEHP). Based on these data the value of 3 µg/l suggested by Staples et al., is used in the risk assessment.

Natural constituents in water may influence the solubility. One study identifies a reduction of the solubility with 15% in well water and 42% in seawater compared to distilled water (Howard et al. 1985). Based on fundamental chemistry the water solubility for DEHP can be assumed to increase in presence of natural occurring dissolved organic matter. Studies describing this are,

however, not available. Monitoring studies indicate that DEHP may occur at higher concentrations (e.g. 92 µg/l in a ground water sample near an industrial landfill, Branzén 2000).

Partition coefficient: n-octanol/water

Log Kow values from 4.8 to 9.6 are available (see **Table 1.1**). Due to the ability of DEHP to form a colloidal dispersion in water, several reported values of log Kow probably are underestimations (Howard et al. 1985). Only results based on HPLC technique or slow-stir methods are therefore assumed to be useful. A value of 7.5 is recommended in a recent review (Staple et al. 1997b). This value is used in the assessment. In the EUSES model the value 7.0 is used (the highest recommended value).

Table 1.1 Available values on water solubility and log Kow on DEHP

Chemical and Physical properties	°C	Comment (Reference)
Water solubility (mg/l)		
0.0006	25°C	Sea water, "generator column" method (Staples et al. 1997)
0.0011 (calc.)	-	(Staples et al. 1997)
0.0026 (calc.)	-	(Staples et al. 1997)
0.003	?	Review recommendation. Used in this assessment (Staples et al. 1997)
Approximately 0.007-0.04	20°C	(BASF AG 1994b)
0.017	22°C	Surface activity method (Thomsen et.al. 2001)
0.029	20°C	(Rippen 1992)
0.041	20°C	(Leyder et al. 1983)
0.045	?	(BASF AG 1989)
0.046	20°C	(OECD 1981)
0.0466	25°C	(ECETOC 1985)
0.0476	15°C	(ECETOC 1985)
0.16	?	Sea water (Howard et al. 1985)
0.28	?°C	(ECETOC 1985)
0.34	25°C	(Howard et al. 1985)
0.34	?	Colloidal suspension (ECETOC, 1985)
0.4	20°C	(ECETOC 1985)
0.6	?°C	(ECETOC 1985)
1.16	?	In sea water (Staples et al. 1997)
1.2	?	In sea water (Staples et al. 1997)
1.3	?°C	(ECETOC 1985)
Solubility ratio:1.0: 0.85: 0.58	?	Distilled water: well water: salt water (Howard et al. 1985)

Table 1.1 continued overleaf

Table 1.1 continued Available values on water solubility and log Kow on DEHP

Chemical and Physical properties	°C	Comment (Reference)
log Kow		
Approximately 4.8	?	(BASF AG 1994b)
4.88	25°C	(Batelle Institut 1982) (BUA 1986)
4.66-5.45	?	Average: 5.11 (Howard et al. 1985)
5.03	?	Calculated (Hoechst AG 1993)
7.14 ± 0.15	?	(Brooke et al 1990)
7.27	?	Measured (Ellington and Floyd 1996)
7.45 ± 0.06	?	Slow-stir apparatus (De Bruijn et al 1989)
7.5	-	Recommend. Used in this assessment (Staples et al. 1997)
7.7	20°C	Measured, RP-HPLC (Condea 1995)
7.86	?	Measured, +- 1.33 (Klein et al. 1988)
7.94	?	"Overestimation", HPLC-method (Howard et al. 1985)
8	20°C	(BASF AG 1987)
9.64	20°C	Calculated (Leyder et.al. 1983)

Other Physico-chemical properties

Surface tension

32.2 mN m⁻¹ at 20°C (Marwedel 1966, in Rippen 2005)

Granulometry

Not applicable (liquid)

Flash point

200°C (DIN 51758) (Riddik et al. 1986)

Autoflammability

Ignition temperature: 370°C (BASF AG 1994a)

Explosivity

Explosion limit: 0.15-0.18 vol.% (BASF AG 1994a; Sorbe 1984 in Rippen 2005)

Explosion limit: 0.3-49 vol.% (Auergesellschaft 1989, in Rippen 2005)

Oxidising properties

Based on DEHP's chemical structure this should be low. "Hazardous reaction influenced by: strong oxidising agents" (Riddik et al. 1986).

Table 1.2 Summary of physico-chemical properties

Property	Value	Reference
Physical state	Colourless oily liquid	see above
Melting point	-55°C or -50°C	see above
Boiling point	230°C at 5 mm Hg 385°C at 1013 hPa	see above
Density	0.986 or 0.984 g/cm ³ at 20°C 0.980-0.985 g/ml	see above
Vapour pressure	0.000034 Pa @ 20°C	see above
Water solubility	3 µg/l @ 20°C	see above
Partition coefficient n-octanol/water (log value)	7.5	see above
Granulometry	N.R.	see above
Conversion factors air	1 ppmv = 16.2 mg/m ³ at 20°C and 1013 hPa	Auergesellschaft 1989 in Rippen 2005
Flash point	200°C	see above
Autoflammability, ignition temperature	370°C	see above
Explosive properties	0.15 - 0.18 vol.% 0.3 – 49 vol%	see above
Oxidizing properties	Not strong oxidising agent	see above
Viscosity, dynamic	81 mPa s at 20°C 58 mPa s at 25°C	IARC 1982 in Rippen 2005 Frische 1979 in Rippen 2005
Henry's constant	see section 3.1.2.2.2	

1.4 CLASSIFICATION

1.4.1 Current classification

Human health:

Classification according to Annex I: Toxic to reproduction, Category 2; R60-61

Environment:

Classification according to
Annex I: None

1.4.2 Proposed classification

Environment

None

Human Health

As adopted in the current classification (above); as given in the 28th ATP of Directive 67/549/EEC.