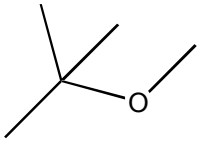
# APPENDIX 1
# General substance information

**IDENTIFICATION OF THE SUBSTANCE**

| | |
|---|---|
| Common chemical name: | Methyl tertiary butyl ether (MTBE) |
| IUPAC / EINECS name: | Propane, 2-methoxy-2- methyl- |
| CAS No.: | 1634-04-4 |
| EINECS No.: | 216-653-1 |
| Molecular formula: | $C_5H_{12}O$ |
| Structural formula: | $H_3C\text{-}O\text{-}C(CH_3)_3$ |
| Molecular weight | 88.15 |

Methyl tertiary butyl ether (MTBE) is an oxygenated aliphatic organic compound, which is a liquid at ambient temperature and pressure. Its structure is:




SMILES notation: [O(C(C)(C)C)C]

**PHYSICO-CHEMICAL PROPERTIES**

A summary of the physico-chemical properties of MTBE are given in Table 1-1 and the key properties for the risk assessment are reviewed in the following sections.

**Table 1-1 Physical and chemical properties of MTBE**

| | |
|---|---|
| Physical state (at NTP) | Colourless liquid |
| Boiling point | 55.2°C |
| Melting point | -108.6°C |
| Flash point | -30°C |
| Autoignition temperature | 425°C |
| Flammability limits in air | 1.5-8.5% |
| Relative density | 0.7405 g/ml at 20°C |
| Vapour pressure | 245 mm of Hg at 25°C, 3.34E+04 Pa at 25°C |
| Refractive index | 1.3690 at 20°C |
| Colour | Colourless |
| Odour | Air: Strong ethereal odour, threshold 0.18mg/m$^3$ (0.24µg.l$^{-1}$, 0.05ppm)<br>Water: threshold 95µg.l$^{-1}$, (0.095ppm) |
| Taste | Water: threshold 134µg.l$^{-1}$, (0.134ppm) |
| Water solubility | 42000 mg.l$^{-1}$ at 25°C (<10% in water, miscible with ethanol and diethyl ether) |
| Partition coefficient n-octanol/water ($log_{10}$) | 1.06 |
| Henry's Law constant | 65.4 Pa/m$^3$/mol |
| Bioaccumulation factor (BCF) | 1.6 (estimated from $log_{10}$Kow), 1.5 (measured for fish) |

Vapour Pressure

Nine measured values of vapour pressure were reported in the HEDSET. The values are 3.34E4 Pa by Ambrose et al. (1976) at 25° C, 2.68E4 Pa at 20° C (Huels Data Sheet, 1993), 2.7E04 Pa at 20° C (ARCO Chemical Company), 4.08E04 Pa at 30° C (ARCO Chemical Company), 5.99E04 Pa at 40° C (ARCO Chemical Company), 2.68E04 Pa at 20° C (ARCO Chemical Company), 4.06E04 Pa at 30° C (ARCO Chemical Company), 6.05E04 Pa at 40° C C (ARCO Chemical Company) and 3.3E04 Pa at 25° C by Daubert and Danner (1985). A value of 3.34E4 Pa was used in the EUSES calculations.

Water Solubility

Data on the solubility of MTBE in water is contradictory in respect of the relationship between solubility and temperature (table 1-2). Results from solubility experiments by Stephenson (1992) show MTBE to exhibit a negative temperature relationship, with solubility increasing as the temperature decreases. This contrasts with the HEDSET solubility data which shows a positive temperature relationship:

**Table 1-2 Comparison of solubility data**

| Temperature ($^{o}$C) | Solubility (g.l$^{-1}$) (Stephenson, 1992) | Solubility (g.l$^{-1}$) HEDSET | HEDSET Reference |
|---|---|---|---|
| 0 | 83 | | |
| 9.7 | 51 | 26 | Huels AG 1993 |
| 19.8 | 42 | 42, 48 | Stephenson, 1992 and Merck Index |
| 25 | | 50 | Huels AG 1993 |
| 29.6 | 31 | | |
| 39.3 | 25 | | |
| 48.6 | 19 | | |

Using the data from the table above, over typical environmental water temperatures (4-18$^{O}$C) in Europe, the solubility in water ranges from about 65 to 40g.l$^{-1}$ (Stephenson, 1992) or about 20 to 45 g.l$^{-1}$ (HEDSET data); these are high solubilities for an organic compound. An intermediate value for water solubility of 42 g.l$^{-1}$ was used for the EUSES risk assessment - this is the approximate solubility at 20$^{o}$C.

Data from BenKinney et al.( 1994) produced during ecotoxicity testing of MTBE, suggests that although it has high solubility in water it is relatively slow to dissolve. Potentially this fact has implications not only for the performance of physicochemical and ecotoxicity tests on MTBE, but also possibly in relation to its likely fate and behaviour in the environment as a consequence of spillages or leaks from storage tanks. However this is the sole reference to such behaviour in the scientific literature.

Since most of the MTBE in use is in gasoline, then the most likely scenario in the environment is that gasoline containing MTBE will come into contact with surface water or groundwater or rainwater. Huttunen (1997) determined the solubility of MTBE in water at 20$^{o}$C using a 1/10 sample to water ratio, both from synthetic mixtures of aliphatic and aromatic hydrocarbons and from gasoline. MTBE, from gasolines containing approximately 1, 4 and 11% by mass of MTBE, dissolved in water to give concentrations of 300, 1100 and 2100 mg.l$^{-1}$. These concentrations are significantly lower than the solubility of pure MTBE in water.

Octanol/Water Partition Coefficient

Four values for the octanol/water partition coefficient (log Kow) are available in the HEDSET. These are a value of 1.06 calculated using a linear free-energy relationship between partition coefficient and the aqueous solubility of organic liquids derived by Hansch (1968). A value of 1.06 was also measured at 23$^{o}$C using the OECD Guideline 107 methodology (Huels AG, 1993). A value of 0.94 was reported by Funasaki *et al.* (1985) and 1.3 by Veith *et al*. (1983). In addition to the values in the HEDSET, a value of 1.43 was calculated using the SRC LOGKOWWIN software based on a structural fragment constant method and an experimentally determined value of 0.94 was reported by Hansch *et al.* (1995). In view of the relatively small range (0.94 to 1.43) covered by these reported values, a value of 1.06 was used in the EUSES based calculations.

Henry's Law Constant

Using the Syracuse Research Corporation (SRC) QSAR software (HENRYWIN) which is based on the fragment constant approach, values of 2.02E-03 atm. m$^{3}$ .mol$^{-1}$ (Bond estimation) and 1.44e-03 atm. m$^{3}$ .mol$^{-1}$ (Group estimation) were calculated. An experimental value of 5.87E-03 atm. m$^{3}$ mol$^{-1}$ was reported by Hine and Mookerjee (1975) and values of 5.28E-03 and 4.33E-03 atm. m$^{3}$ .mol$^{-1}$ by Robbins et al. (1993) – all at 25$^{o}$ C. No value was entered to EUSES, so the slightly lower EUSES calculated value (derived from water solubility and vapour pressure) of 70.1 Pa.m$^{3}$.mol$^{-1}$ (6.9E-04 atm. m$^{3}$ mol$^{-1}$) was used in the assessment.

Taste and Odour

MTBE is a volatile liquid at normal room temperature and pressure and has a strong ethereal odour in air, with a threshold concentration of 0.18mg/m3 (0.24μg.l$^{-1}$, 0.05ppm).

MTBE imparts a pronounced taste and odour to water at very low concentrations and this has the beneficial effect that exposure of consumers to toxic quantities via consumption of water is unlikely. However, because of the wide range of sensitivity of response of the human population to tastes and odours and different approaches to setting guideline values for organoleptic parameters (Fawell and Young, 1997), reported odour thresholds can vary considerably.

Vertrano (1993) reported an odour detection threshold in water of 95μg.l$^{-1}$ and a taste threshold in water of 134μg.l$^{-1}$. The Oxygenated Fuels Association in the US commissioned an extensive test on the aesthetic properties of MTBE in water (Pirnie, 1998) using an odour panel of 57 participants. The results of the study supported the setting of a Secondary Maximum Contaminant Limit (SMCL – an advisory guideline set for aesthetic, non-health effect parameters by the USEPA) of 15μg.l$^{-1}$ for taste and odour in drinking water. The actual USEPA advisory level set for taste and odour considerations in drinking water is 20-40 μg.l$^{-1}$, which is reported to provide a large margin of safety from toxic effects (USEPA, 1997). Also in the US, the California EPA has recently adopted an SMCL of 5 μg.l$^{-1}$ (OEHHA, 1999). A study in the UK by Fawell and Young (1997) suggested a guidance value for taste and odour in drinking water of 10 or 34 μg.l$^{-1}$ dependent on the considerations applied to the dataset used to establish the taste and odour threshold. The health implications of the taste and odour properties of MTBE are discussed in more detail in Section 4 (Human Health).

**PURITY/IMPURITIES, ADDITIVES**

| | |
|---|---|
| Degree of purity: | >98% w/w |
| Identity and percentage of impurities: | tertiary butyl alcohol (<1% w/w)<br>2,4,4-trimethylpent-1-ene (<1% w/w)<br>triisobutylene (<0.5% w/w)<br>methanol (<0.5% w/w)<br>C4-C6 hydrocarbons (<1% w/w) |
| Identity and percentage of necessary additives: | Not applicable. |

**CLASSIFICATION ACCORDING TO ANNEX I**

Classification according to Annex I of Directive 67/548/EEC: R11/38

R11 - Highly flammable, R38 – Irritant

**General Note:** the HEDSET contains several values for some of the parameters, but only a single value can be input to EUSES so some selection criteria are required to decide which values to use. In general, where the difference between the values was minimal (1-2%), then the lowest value was selected. Where the difference between the values was greater than 1-2%, then an intermediate value was selected.