1-*tert*-BUTOXYPROPAN-2-OL

1. Exposure Data

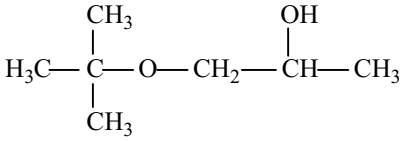
1.1 Chemical and physical data

The chemical that is the subject of this monograph, 1-*tert*-butoxypropan-2-ol, is commonly known as propylene glycol mono-*tert*-butyl ether. However, the latter name is non-specific and could also refer to 2-*tert*-butoxypropan-1-ol or to the mixture of the 1- and 2-isomers (also called α- and β-isomers, respectively). Thus, the name 1-*tert*-butoxypropan-2-ol was chosen for this monograph to avoid ambiguity.

1.1.1 *Nomenclature*

From National Library of Medicine (2004)
Chem. Abstr. Serv. Reg. No.: 57018-52-7
Deleted CAS Reg. No.: 136579-67-4
Chem. Abstr. Name: 1-(1,1-Dimethylethoxy)-2-propanol
Synonyms: 1-*tert*-Butoxy-2-propanol; 1-methyl-2-*tert*-butoxyethanol; propylene glycol 1-(*tert*-butyl ether); propylene glycol mono-*tert*-butyl ether, α-isomer

1.1.2 *Structural and molecular formulae and relative molecular mass*



$C_7H_{16}O_2$ Relative molecular mass: 132.2

1.1.3 *Chemical and physical properties of the pure substance*

From Lyondell Chemical Co. (2004), unless otherwise specified
(*a*) *Description*: Colourless, combustible liquid with a characteristic odour similar to that of eucalyptus

(*b*) *Boiling-point*: 151 °C (Boatman, 2001)
(*c*) *Melting-point*: –27 °C (Staples & Davis, 2002)
(*d*) *Density*: Specific gravity, 0.87 at 25/4 °C (Boatman, 2001)
(*e*) *Spectroscopy*: Infrared, nuclear magnetic resonance (proton and carbon-13) and mass spectral data have been reported (National Toxicology Program, 2004a).
(*f*) *Solubility*: Soluble in water (18% at 20 °C); miscible with many organic solvents; solubility in water is increased by the addition of low-molecular-weight alcohols and other water-miscible glycol ethers.
(*g*) *Volatility*: Vapour pressure, 2.7 mm Hg at 25 °C (93 Pa at 25 °C; Staples & Davis, 2002); flash-point (Tag closed-cup), 45 °C; flammability limits (lower/upper vol. %), 1.8/6.8
(*h*) *Octanol/water partition coefficient (P)*: log P, 0.87 (Staples & Davis, 2002)
(*i*) *Conversion factor*: $mg/m^3 = 5.4 \times ppm$[1]

1.1.4 *Technical products and impurities*

Trade names for 1-*tert*-butoxypropan-2-ol include Arcosolv® PTB. It is commercially available in the USA with the following specifications: purity, min. 99.0%; specific gravity (at 25/25 °C), 0.870–0.874; acidity (% wt as acetic acid, max.), 0.03; and water (% wt, max.), 0.25 (Lyondell Chemical Co., 2004). Potential impurities include: 2-*tert*-butoxypropan-1-ol (β-isomer; < 0.5%), propylene glycol di-*tert*-butyl ether, propylene glycol, *tert*-butanol and isobutylene (Knifton, 1994).

1.1.5 *Analysis*

1-*tert*-Butoxypropan-2-ol has been quantified in commercial technical products using gas chromatography (GC) with mass spectrometry and GC with flame ionization detection (FID). It has also been determined in air using GC/FID (National Toxicology Program, 2004a).

1.2 Production and use

Glycol ethers began to be used in the 1930s and some have been in general use for nearly 50 years. They form a varied family of more than 30 solvents that commonly dissolve in both water and oil. For this reason, they are very useful in numerous industrial (paints, pharmaceutical industry, inks) and consumer (cosmetics, detergents) applications. Traditionally, a distinction is made between two main groups of glycol ethers: the E series and the P series, which derive from the name of the chemical substances that serve as a starting point for their production (ethylene and propylene, respectively). In each series,

[1] Calculated from: $mg/m^3 = (\text{relative molecular mass}/24.45) \times ppm$, assuming normal temperature (25 °C) and pressure (103.5 kPa)

different derivatives have been developed to provide the properties of solubility, volatility, compatibility and inflammability that are required for different uses. Since the mid-1980s, concerns about the toxic effects of the E-series glycol ethers have stimulated the development of P-series products as potential substitutes. 1-*tert*-Butoxypropan-2-ol is one of several monoalkyl ethers of propylene glycol that is finding increasing use as a replacement for the E-series glycol ethers (Begley, 1986; Chinn *et al*, 2000; Oxygenated Solvents Producers Association, 2004).

1.2.1 *Production*

The ethers of propylene glycol are prepared commercially by reacting propylene oxide with the alcohol of choice in the presence of a catalyst. They may also be prepared by direct alkylation of the selected glycol with an appropriate alkylating agent such as dialkyl sulfate in the presence of an alkali. Commercial synthesis typically yields products that are mixtures of the α- and β-isomers. The α-isomer has the ether linkage on the terminal hydroxyl group of propylene glycol, while the β-isomer has the ether linkage on the secondary hydroxyl group. The α-isomer is thermodynamically favoured and is the predominant ether formed. By controlling the conditions of synthesis, the proportion of α-isomer may be enhanced to constitute more than 99% of the end-product (Boatman, 2001).

1-*tert*-Butoxypropan-2-ol is generally manufactured by reacting isobutylene with excess propylene glycol in the presence of a solid-resin etherification catalyst. The product is then distilled to produce ≥ 99% of the α-isomer, 1-*tert*-butoxypropan-2-ol (Gupta, 1987). The commercial product contains > 99.5% of the α-isomer (1-*tert*-butoxypropan-2-ol) (Staples & Davies, 2002).

Available information indicates that 1-*tert*-butoxypropan-2-ol was produced by one company in the USA (Chemical Information Services, 2004; Lyondell Chemical Co, 2004). Estimated production of 1-*tert*-butoxypropan-2-ol in the USA between 1989 and 1999 is shown in Table 1 (Chinn *et al*., 2000).

Table 1. Production of 1-*tert*-butoxypropan-2-ol from 1989 to 1999 in the USA (tonnes)

1989	1991	1993	1995	1997	1999
230	1100	1400	1800	1800	2300

From Chinn *et al*. (2000)

1.2.2 *Use*

Butyl ethers have limited solubility in water but are miscible with most organic solvents, which favours their use as coupling, coalescing and dispersing agents. Butyl glycol ethers have been used as solvents for surface coatings, inks, lacquers, paints, resins, dyes, agricultural chemicals and other oils and greases.

1-*tert*-Butoxypropan-2-ol is a better coupling agent and has higher electrolyte solubility than 2-butoxyethanol. It is used commercially as a solvent in water-reducible coatings and in a variety of commercial cleaner formulations including all-purpose, glass- and hard surface-cleaning products. It is also used in inks, adhesives and agricultural, electronic, cosmetic and textile products (Boatman, 2001; Lyondell Chemical Co., 2004).

1.3 Occurrence

1.3.1 *Natural occurrence*

1-*tert*-Butoxypropan-2-ol is not known to occur as a natural product.

1.3.2 *Occupational exposure*

There is a potential for occupational exposure to 1-*tert*-butoxypropan-2-ol mainly via inhalation and dermal absorption during its production and use in a variety of products. Because 1-*tert*-butoxypropan-2-ol is readily absorbed through the skin and has a relatively low vapour pressure, the dermal route may be predominant or may contribute significantly to overall exposure. No data on exposure were available to the Working Group; however, exposure during the manufacturing process is thought to be low since it is largely enclosed (Boatman, 2001).

1.3.3 *Consumer exposure*

1-*tert*-Butoxypropan-2-ol is used in a variety of products and consumer exposure may potentially occur during the handling or use of products that contain this chemical (Boatman, 2001). However, no data were available on levels of consumer exposure.

1.3.4 *Environmental occurrence*

No information was available to the Working Group on environmental exposure to 1-*tert*-butoxypropan-2-ol.

1.4 Regulations and guidelines

No occupational exposure limits (Boatman, 2001) or other occupational or environmental regulations or guidelines have been established for 1-*tert*-butoxypropan-2-ol.