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Dibutyl ether

Dibutyl ether is a chemical compound belonging to the ether family with the molecular formula of $C_8H_{18}O$. It is colorless, volatile, and flammable liquid and has peculiar ethereal smell.

Liquid dibutyl ether is lighter than water. On the other hand, the vapor is heavier than air. It is not soluble in water, but it is soluble in acetone and many other organic solvents. Due to this property, dibutyl ether is used as solvent in various chemical reactions and processes. For example, phenyllithium is commercially available as a ca. 1.8 M solution in dibutyl ether.

Because of the formation of peroxides, it should be protected from heat, light and air.

Contents

Synthesis

Dibutyl ether is obtained from dehydration of 1-butanol with sulfuric acid as a catalyst and dehydrating agent:

$$2C_4H_9OH \rightarrow C_8H_{18}O + H_2O$$

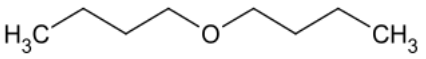
Industrially, dibutyl ether can be obtained by dehydration of 1-butanol on alumina at 300 °C.

Reactions

This compound is generally stable to oxidation, reduction, and base. Strong acids like HI and HBr can cleave this ether. In the presence of oxygen, dibutyl ether is oxidized to a peroxide or hydroperoxide.

Applications

Dibutyl ether



Names	
Preferred IUPAC name	1-Butoxybutane
Other names	▪ Di-*n*-butyl ether ▪ Butyl ether ▪ *n*-Butyl ether
Identifiers	
CAS Number	142-96-1 (https://commonchemistry.cas.org/detail?cas_rn=142-96-1) ✓
3D model (JSmol)	Interactive image (https://chemapps.stolaf.edu/jmol/jmol.php?model=CCCCOCCCC)
ChemSpider	8569 (http://www.chemspider.com/Chemical-Structure.8569.html)
ECHA InfoCard	100.005.069 (https://echa.europa.eu/substance-information/-/substanceinfo/100.005.069)
PubChem CID	8909 (https://pubchem.ncbi.nlm.nih.gov/compound/8909)
UNII	PBM2R52P5G (https://fdasis.nlm.nih.gov/srs/srsdirect.jsp?regno=PBM2

- Solvent for Grignard syntheses
- Solvent for fats, oils, organic acids, alkaloids, natural and synthetic resins
- For manufacturing of pesticides (e.g. Cyhexatin)

References

1. Record (https://gestis.dguv.de/data?name=028060&lang=en) in the GESTIS Substance Database of the Institute for Occupational Safety and Health

	R52P5G) ✓
CompTox Dashboard (EPA)	DTXSID1022007 (https://comptox.epa.gov/dashboard/DTXSID1022007)
InChI	
InChI=1S/C8H18O/c1-3-5-7-9-8-6-4-2/h3-8H2,1-2H3 Key: DURPTKYDGMDSBL-UHFFFAOYSA-N	
InChI=1/C8H18O/c1-3-5-7-9-8-6-4-2/h3-8H2,1-2H3 Key: DURPTKYDGMDSBL-UHFFFAOYAH	
SMILES	
CCCCOCCCC	
Properties	
Chemical formula	$C_8H_{18}O$
Molar mass	130.231 g·mol^{-1}
Appearance	Colorless liquid[1]
Odor	Fruity[1]
Density	0.77 g/cm^3 (20 °C)[1]
Melting point	−95 °C (−139 °F; 178 K)[1]
Boiling point	141 °C (286 °F; 414 K)[1]
Solubility in water	0.3 g/L[1]
Refractive index (n_D)	1.3992
Viscosity	0.741 cP (15 °C)
Structure	
Dipole moment	1.18 D
Hazards	
Flash point	25 °C (77 °F; 298 K)
Autoignition temperature	175 °C (347 °F; 448 K)[1]
Lethal dose or concentration (LD, LC):	

LD_{50} (median dose)	7400 mg/kg (oral, rat)[1]
Except where otherwise noted, data are given for materials in their standard state (at 25 °C [77 °F], 100 kPa). Infobox references	

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