# 1-Tert-butoxybutane

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|---|---|
| **Other names:** | 1,1-dimethyl-1-butoxyethane<br>1-(1,1-dimethylethoxy)butane<br>1-butyl tert-butyl ether<br>2,2-dimethyl-3-oxaheptane<br>butane, 1-(1,1-dimethylethoxy)-<br>butyl 1,1-dimethylethyl ether<br>butyl tert-butyl ether<br>ethane, 1-butoxy-1,1-dimethyl-<br>ether, butyl tert-butyl<br>n-butyl tert-butyl ether<br>tert-butyl butyl ether |
| **Inchi:** | InChI=1S/C8H18O/c1-5-6-7-9-8(2,3)4/h5-7H2,1-4H3 |
| **InchiKey:** | JJNQHLLBFBGKEL-UHFFFAOYSA-N |
| **Formula:** | C8H18O |
| **SMILES:** | CCCCOC(C)(C)C |
| **Mol. weight [g/mol]:** | 130.23 |
| **CAS:** | 1000-63-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -5317.30 ± 1.50 | kJ/mol | NIST Webbook |
| gf | -85.68 | kJ/mol | Joback Method |
| hf | -361.00 ± 1.90 | kJ/mol | NIST Webbook |
| hfl | -403.30 ± 1.90 | kJ/mol | NIST Webbook |
| hfus | 10.25 | kJ/mol | Joback Method |
| hvap | 42.30 ± 0.30 | kJ/mol | NIST Webbook |
| hvap | 41.60 ± 0.20 | kJ/mol | NIST Webbook |
| hvap | 42.33 ± 0.25 | kJ/mol | NIST Webbook |
| hvap | 43.20 | kJ/mol | NIST Webbook |
| log10ws | -2.37 | | Crippen Method |
| logp | 2.602 | | Crippen Method |
| mcvol | 129.450 | ml/mol | McGowan Method |
| pc | 2540.49 | kPa | Joback Method |
| rinpol | 803.00 | | NIST Webbook |
| rinpol | 796.20 | | NIST Webbook |
| rinpol | 796.00 | | NIST Webbook |
| rinpol | 803.00 | | NIST Webbook |

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|---|---|---|---|
| tb | 397.15 ± 4.00 | K | NIST Webbook |
| tb | 397.00 ± 2.00 | K | NIST Webbook |
| tb | 395.65 | K | Isobaric vapor liquid equilibria of 1,1-dimethylethoxy-butane + methanol or ethanol +water at 101.32 kPa |
| tc | 576.09 | K | Joback Method |
| tf | 204.57 | K | Joback Method |
| vc | 0.490 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 335.39 | J/mol×K | 576.09 | Joback Method |
| cpg | 258.96 | J/mol×K | 401.63 | Joback Method |
| cpg | 273.09 | J/mol×K | 430.71 | Joback Method |
| cpg | 286.65 | J/mol×K | 459.78 | Joback Method |
| cpg | 299.64 | J/mol×K | 488.86 | Joback Method |
| cpg | 312.08 | J/mol×K | 517.94 | Joback Method |
| cpg | 323.99 | J/mol×K | 547.02 | Joback Method |
| dvisc | 0.0002404 | Pa×s | 401.63 | Joback Method |
| dvisc | 0.0073558 | Pa×s | 204.57 | Joback Method |
| dvisc | 0.0028037 | Pa×s | 237.41 | Joback Method |
| dvisc | 0.0013510 | Pa×s | 270.26 | Joback Method |
| dvisc | 0.0007626 | Pa×s | 303.10 | Joback Method |
| dvisc | 0.0004814 | Pa×s | 335.94 | Joback Method |
| dvisc | 0.0003298 | Pa×s | 368.79 | Joback Method |
| hvapt | 38.30 | kJ/mol | 376.50 | NIST Webbook |
| hvapt | 41.70 | kJ/mol | 345.00 | NIST Webbook |
| rfi | 1.39170 | | 298.10 | PHYSICAL AND EXCESS PROPERTIES OF BINARY AND TERNARY MIXTURES OF 1,1-DIMETHYLETHOXY-BUTANE, METHANOL, ETHANOL AND WATER AT 298.15K. |

# Sources

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| **Thermodynamic Analysis of the Experimental Equilibria for the Liquid-Phase Etherification of Isobutene with C1 to C4 Linear Primary Alcohols:** | https://www.doi.org/10.1021/acs.jced.5b00557 |
| **PHYSICAL AND EXCESS PROPERTIES OF BINARY AND TERNARY MIXTURES CONTAINING METHYLETHOXY-BUTANE, METHANOL, ETHANOL AND WATER AT 298.15K:** | https://www.doi.org/10.1016/j.tca.2005.04.030 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers:** | https://www.doi.org/10.1021/je049823k |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1000631&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Isobaric vapor liquid equilibria of 1,1-dimethylethoxy-butane + methanol or ethanol +water at 101.32 kPa:** | https://www.doi.org/10.1016/j.fluid.2007.01.038 |

# Legend

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|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rfi:** | Refractive Index |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |