# Propane, 1,1-diethoxy-2-methyl-

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|---|---|
| **Other names:** | Isobutyraldehyde, diethyl acetal |
| | Isobutanal diethyl acetal |
| | Isobutylaldehyde diethyl acetal |
| | 1,1-Diethoxy-2-methylpropane |
| | 1,1-Diethoxyisobutane |
| **Inchi:** | InChI=1S/C8H18O2/c1-5-9-8(7(3)4)10-6-2/h7-8H,5-6H2,1-4H3 |
| **InchiKey:** | KZDFOVZPOBSHDH-UHFFFAOYSA-N |
| **Formula:** | C8H18O2 |
| **SMILES:** | CCOC(OCC)C(C)C |
| **Mol. weight [g/mol]:** | 146.23 |
| **CAS:** | 1741-41-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -198.40 | kJ/mol | Joback Method |
| hf | -483.45 | kJ/mol | Joback Method |
| hfus | 11.81 | kJ/mol | Joback Method |
| hvap | 37.45 | kJ/mol | Joback Method |
| log10ws | -1.71 | | Crippen Method |
| logp | 2.042 | | Crippen Method |
| mcvol | 135.320 | ml/mol | McGowan Method |
| pc | 2490.03 | kPa | Joback Method |
| rinpol | 858.00 | | NIST Webbook |
| rinpol | 859.00 | | NIST Webbook |
| rinpol | 865.00 | | NIST Webbook |
| rinpol | 858.00 | | NIST Webbook |
| rinpol | 859.00 | | NIST Webbook |
| rinpol | 850.00 | | NIST Webbook |
| rinpol | 859.00 | | NIST Webbook |
| rinpol | 830.00 | | NIST Webbook |
| rinpol | 859.00 | | NIST Webbook |
| rinpol | 859.00 | | NIST Webbook |
| ripol | 969.00 | | NIST Webbook |
| ripol | 977.00 | | NIST Webbook |
| ripol | 977.00 | | NIST Webbook |
| ripol | 1000.00 | | NIST Webbook |
| ripol | 962.00 | | NIST Webbook |

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|---|---|---|---|
| ripol | 970.00 | | NIST Webbook |
| ripol | 976.00 | | NIST Webbook |
| ripol | 969.00 | | NIST Webbook |
| tb | 411.00 ± 4.00 | K | NIST Webbook |
| tc | 597.88 | K | Joback Method |
| tf | 194.38 | K | Joback Method |
| vc | 0.507 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 282.44 | J/mol×K | 426.40 | Joback Method |
| cpg | 295.62 | J/mol×K | 454.98 | Joback Method |
| cpg | 308.43 | J/mol×K | 483.56 | Joback Method |
| cpg | 320.85 | J/mol×K | 512.14 | Joback Method |
| cpg | 332.88 | J/mol×K | 540.72 | Joback Method |
| cpg | 344.52 | J/mol×K | 569.30 | Joback Method |
| cpg | 355.77 | J/mol×K | 597.88 | Joback Method |
| dvisc | 0.0084710 | Pa×s | 194.38 | Joback Method |
| dvisc | 0.0026002 | Pa×s | 233.05 | Joback Method |
| dvisc | 0.0011171 | Pa×s | 271.72 | Joback Method |
| dvisc | 0.0005924 | Pa×s | 310.39 | Joback Method |
| dvisc | 0.0003615 | Pa×s | 349.06 | Joback Method |
| dvisc | 0.0002435 | Pa×s | 387.73 | Joback Method |
| dvisc | 0.0001762 | Pa×s | 426.40 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C1741419&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

# Legend

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