# 7-Oxabicyclo[2.2.1]heptane

| | |
|---|---|
| **Other names:** | 7-Oxanorbornane |
| | Cyclohexane, 1,4-epoxy- |
| | Cyclohexane, 3,6-endoxo- |
| | 1,4-Epoxycyclohexane |
| | 1,4-Oxycyclohexane |
| | 3,6-Endooxycyclohexane |
| | 3,6-Endoxocyclohexane |
| | Bicyclo[2.2.1]heptane, 7-oxa- |
| **Inchi:** | InChI=1S/C6H10O/c1-2-6-4-3-5(1)7-6/h5-6H,1-4H2 |
| **InchiKey:** | YPWFNLSXQIGJCK-UHFFFAOYSA-N |
| **Formula:** | C6H10O |
| **SMILES:** | C1CC2CCC1O2 |
| **Mol. weight [g/mol]:** | 98.14 |
| **CAS:** | 279-49-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 844.20 | kJ/mol | NIST Webbook |
| basg | 816.80 | kJ/mol | NIST Webbook |
| chl | -3566.30 ± 1.50 | kJ/mol | NIST Webbook |
| chl | -3566.30 ± 1.50 | kJ/mol | NIST Webbook |
| gf | 22.92 | kJ/mol | Joback Method |
| hf | -159.73 | kJ/mol | Joback Method |
| hfl | -223.90 ± 2.00 | kJ/mol | NIST Webbook |
| hfus | 13.44 | kJ/mol | Joback Method |
| hvap | 33.46 | kJ/mol | Joback Method |
| ie | 9.57 ± 0.02 | eV | NIST Webbook |
| log10ws | -1.43 | | Crippen Method |
| logp | 1.328 | | Crippen Method |
| mcvol | 79.550 | ml/mol | McGowan Method |
| pc | 4339.67 | kPa | Joback Method |
| tb | 381.38 | K | Joback Method |
| tc | 586.65 | K | Joback Method |
| tf | 216.31 | K | Joback Method |
| vc | 0.298 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 151.20 | J/mol×K | 381.38 | Joback Method |
| cpg | 165.70 | J/mol×K | 415.59 | Joback Method |
| cpg | 179.24 | J/mol×K | 449.80 | Joback Method |
| cpg | 191.89 | J/mol×K | 484.02 | Joback Method |
| cpg | 203.68 | J/mol×K | 518.23 | Joback Method |
| cpg | 214.68 | J/mol×K | 552.44 | Joback Method |
| cpg | 224.93 | J/mol×K | 586.65 | Joback Method |
| dvisc | 0.0009627 | Pa×s | 216.31 | Joback Method |
| dvisc | 0.0008301 | Pa×s | 243.82 | Joback Method |
| dvisc | 0.0007377 | Pa×s | 271.33 | Joback Method |
| dvisc | 0.0006699 | Pa×s | 298.85 | Joback Method |
| dvisc | 0.0006183 | Pa×s | 326.36 | Joback Method |
| dvisc | 0.0005779 | Pa×s | 353.87 | Joback Method |
| dvisc | 0.0005454 | Pa×s | 381.38 | Joback Method |
| hfust | 0.71 | kJ/mol | 244.00 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 392.20 | K | 95.10 | NIST Webbook |

# Sources

**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

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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C279492&Units=SI

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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