# 2,2'-Bioxirane

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|---|---|
| **Other names:** | Butane, 1,2:3,4-diepoxy- |
| | Bioxirane |
| | Butadiene diepoxide |
| | Butadiene dioxide |
| | Butane diepoxide |
| | Diepoxybutane |
| | Dioxybutadiene |
| | 1,1'-Bi[ethylene oxide] |
| | 1,2,3,4-Diepoxybutane |
| | 1,2:3,4-Diepoxybutane |
| | Bioxiran |
| | CB 1181 |
| | M 8838 |
| | R 181 |
| | Threitol, 1,2:3,4-dianhydro- |
| | Butadiendioxyd |
| | 1,3-Butadiene diepoxide |
| | DEB |
| | ENT-26592 |
| | Rcra waste number U085 |
| | NSC 629 |
| **Inchi:** | InChI=1S/C4H6O2/c1-3(5-1)4-2-6-4/h3-4H,1-2H2 |
| **InchiKey:** | ZFIVKAOQEXOYFY-UHFFFAOYSA-N |
| **Formula:** | C4H6O2 |
| **SMILES:** | C1OC1C1CO1 |
| **Mol. weight [g/mol]:** | 86.09 |
| **CAS:** | 1464-53-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -67.94 | kJ/mol | Joback Method |
| hf | -244.29 | kJ/mol | Joback Method |
| hfus | 18.34 | kJ/mol | Joback Method |
| hvap | 33.34 | kJ/mol | Joback Method |
| log10ws | 0.32 | | Crippen Method |
| logp | -0.216 | | Crippen Method |

| | | | |
|---|---|---|---|
| mcvol | 57.240 | ml/mol | McGowan Method |
| pc | 5406.57 | kPa | Joback Method |
| tb | 358.30 | K | Joback Method |
| tc | 558.39 | K | Joback Method |
| tf | 223.86 | K | Joback Method |
| vc | 0.215 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 109.07 | J/mol×K | 358.30 | Joback Method |
| cpg | 119.63 | J/mol×K | 391.65 | Joback Method |
| cpg | 129.41 | J/mol×K | 425.00 | Joback Method |
| cpg | 138.46 | J/mol×K | 458.35 | Joback Method |
| cpg | 146.83 | J/mol×K | 491.69 | Joback Method |
| cpg | 154.56 | J/mol×K | 525.04 | Joback Method |
| cpg | 161.70 | J/mol×K | 558.39 | Joback Method |
| dvisc | 0.0007038 | Pa×s | 223.86 | Joback Method |
| dvisc | 0.0006732 | Pa×s | 246.27 | Joback Method |
| dvisc | 0.0006488 | Pa×s | 268.67 | Joback Method |
| dvisc | 0.0006288 | Pa×s | 291.08 | Joback Method |
| dvisc | 0.0006122 | Pa×s | 313.49 | Joback Method |
| dvisc | 0.0005981 | Pa×s | 335.89 | Joback Method |
| dvisc | 0.0005861 | Pa×s | 358.30 | Joback Method |

# 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=C1464535&Units=SI

# Legend

**cpg:** Ideal gas heat capacity

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|---|---|
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |