# 2,2-DI-(2'-CHLOROETHOXY)-ETHANE

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|---|---|
| **Other names:** | 1,1'-(Ethylidene)bis(oxy)bis(2-chloroethane) |
| | 1,1-Bis(2-chloroethoxy)ethane |
| | Di(2-chloroethyl)acetal |
| | Ethane, 1,1'-(ethylidene)bis(oxy)bis(2-chloro- |
| | Ethane,-1,1-di(2-chloroehtoxy) |
| | bis(2-chloroethyl)acetaldehyde acetal |
| **Inchi:** | InChI=1S/C6H12Cl2O2/c1-6(9-4-2-7)10-5-3-8/h6H,2-5H2,1H3 |
| **InchiKey:** | KHNOWHUSVXGGLG-UHFFFAOYSA-N |
| **Formula:** | C6H12Cl2O2 |
| **SMILES:** | CC(OCCCl)OCCCl |
| **Mol. weight [g/mol]:** | 187.07 |
| **CAS:** | 14689-97-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -519.74 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 18.54 | kJ/mol | Joback Method |
| hvap | 52.50 | kJ/mol | Cheméo Relay (1.0) |
| ie | 10.16 | eV | Cheméo Relay (1.0) |
| log10ws | -1.48 | | Cheméo Relay (1.0) |
| logp | 1.843 | | Crippen Method |
| mcvol | 131.620 | ml/mol | McGowan Method |
| pc | 2787.66 | kPa | Joback Method |
| tb | 460.83 | K | Cheméo Relay (1.0) |
| tc | 644.34 | K | Cheméo Relay (1.0) |
| tf | 217.66 | K | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 303.39 | J/mol×K | 608.69 | Joback Method |
| cpg | 311.76 | J/mol×K | 639.24 | Joback Method |
| cpg | 266.52 | J/mol×K | 486.49 | Joback Method |
| cpg | 276.23 | J/mol×K | 517.04 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 285.62 | J/mol×K | 547.59 | Joback Method |
| cpg | 294.67 | J/mol×K | 578.14 | Joback Method |
| cpg | 256.50 | J/mol×K | 455.94 | Joback Method |
| dvisc | 0.0009509 | Pa×s | 316.43 | Joback Method |
| dvisc | 0.0017107 | Pa×s | 281.56 | Joback Method |
| dvisc | 0.0036333 | Pa×s | 246.68 | Joback Method |
| dvisc | 0.0005940 | Pa×s | 351.31 | Joback Method |
| dvisc | 0.0004039 | Pa×s | 386.19 | Joback Method |
| dvisc | 0.0002928 | Pa×s | 421.06 | Joback Method |
| dvisc | 0.0002230 | Pa×s | 455.94 | Joback Method |
| hvapt | 59.40 | kJ/mol | 407.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.24851e+01 |
| Coeff. B | -3.97012e+03 |
| Coeff. C | -3.61200e+01 |
| Temperature range (K), min. | 329.00 |
| Temperature range (K), max. | 589.55 |

# Sources

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

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

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

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

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C14689975&Units=SI

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **hf:** | 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 |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |