# «alpha»-Chloroethyl chloroformate

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|---|---|
| **Other names:** | 1-Chloroethyl chloroformate |
| | Carbonochloridic acid, 1-chloroethyl ester |
| **Inchi:** | InChI=1S/C3H4Cl2O2/c1-2(4)7-3(5)6/h2H,1H3 |
| **InchiKey:** | QOPVNWQGBQYBBP-UHFFFAOYSA-N |
| **Formula:** | C3H4Cl2O2 |
| **SMILES:** | CC(Cl)OC(=O)Cl |
| **Mol. weight [g/mol]:** | 142.97 |
| **CAS:** | 50893-53-3 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -285.84 | kJ/mol | Joback Method |
| hf | -386.81 | kJ/mol | Joback Method |
| hfus | 11.18 | kJ/mol | Joback Method |
| hvap | 39.81 | kJ/mol | Joback Method |
| log10ws | -1.83 | | Crippen Method |
| logp | 1.947 | | Crippen Method |
| mcvol | 85.050 | ml/mol | McGowan Method |
| pc | 4294.29 | kPa | Joback Method |
| tb | 418.75 | K | Joback Method |
| tc | 620.11 | K | Joback Method |
| tf | 240.57 | K | Joback Method |
| vc | 0.320 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 137.02 | J/mol×K | 418.75 | Joback Method |
| cpg | 161.59 | J/mol×K | 586.55 | Joback Method |
| cpg | 157.07 | J/mol×K | 552.99 | Joback Method |
| cpg | 152.35 | J/mol×K | 519.43 | Joback Method |
| cpg | 147.43 | J/mol×K | 485.87 | Joback Method |
| cpg | 142.32 | J/mol×K | 452.31 | Joback Method |
| cpg | 165.90 | J/mol×K | 620.11 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003593 | Pa×s | 418.75 | Joback Method |
| dvisc | 0.0004588 | Pa×s | 389.05 | Joback Method |
| dvisc | 0.0006101 | Pa×s | 359.36 | Joback Method |
| dvisc | 0.0008540 | Pa×s | 329.66 | Joback Method |
| dvisc | 0.0012778 | Pa×s | 299.96 | Joback Method |
| dvisc | 0.0020888 | Pa×s | 270.27 | Joback Method |
| dvisc | 0.0038551 | Pa×s | 240.57 | Joback Method |

# Sources

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|---|---|
| **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=C50893533&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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