# 2,2-dichloroethyl heptanoate

**Inchi:** InChI=1S/C9H16Cl2O2/c1-2-3-4-5-6-9(12)13-7-8(10)11/h8H,2-7H2,1H3
**InchiKey:** KKDZZVNLJUMCED-UHFFFAOYSA-N
**Formula:** C9H16Cl2O2
**SMILES:** CCCCCCC(=O)OCC(Cl)Cl
**Mol. weight [g/mol]:** 227.13

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -235.32 | kJ/mol | Joback Method |
| hf | -510.65 | kJ/mol | Joback Method |
| hfus | 26.72 | kJ/mol | Joback Method |
| hvap | 53.17 | kJ/mol | Joback Method |
| log10ws | -3.37 | | Crippen Method |
| logp | 3.304 | | Crippen Method |
| mcvol | 169.590 | ml/mol | McGowan Method |
| pc | 2263.26 | kPa | Joback Method |
| rinpol | 1378.00 | | NIST Webbook |
| rinpol | 1388.00 | | NIST Webbook |
| rinpol | 1392.00 | | NIST Webbook |
| rinpol | 1384.00 | | NIST Webbook |
| rinpol | 1381.00 | | NIST Webbook |
| rinpol | 1378.00 | | NIST Webbook |
| ripol | 1850.00 | | NIST Webbook |
| ripol | 1900.00 | | NIST Webbook |
| ripol | 1860.00 | | NIST Webbook |
| ripol | 1900.00 | | NIST Webbook |
| ripol | 1854.00 | | NIST Webbook |
| ripol | 1886.00 | | NIST Webbook |
| ripol | 1852.00 | | NIST Webbook |
| ripol | 1869.00 | | NIST Webbook |
| ripol | 1850.00 | | NIST Webbook |
| tb | 556.03 | K | Joback Method |
| tc | 743.61 | K | Joback Method |
| tf | 308.19 | K | Joback Method |
| vc | 0.655 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 380.33 | J/mol×K | 556.03 | Joback Method |
| cpg | 437.41 | J/mol×K | 712.35 | Joback Method |
| cpg | 427.10 | J/mol×K | 681.08 | Joback Method |
| cpg | 416.25 | J/mol×K | 649.82 | Joback Method |
| cpg | 404.84 | J/mol×K | 618.56 | Joback Method |
| cpg | 392.87 | J/mol×K | 587.29 | Joback Method |
| cpg | 447.18 | J/mol×K | 743.61 | Joback Method |
| dvisc | 0.0002166 | Pa×s | 556.03 | Joback Method |
| dvisc | 0.0002852 | Pa×s | 514.72 | Joback Method |
| dvisc | 0.0003940 | Pa×s | 473.42 | Joback Method |
| dvisc | 0.0005790 | Pa×s | 432.11 | Joback Method |
| dvisc | 0.0009231 | Pa×s | 390.80 | Joback Method |
| dvisc | 0.0016431 | Pa×s | 349.50 | Joback Method |
| dvisc | 0.0034137 | Pa×s | 308.19 | 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=R30620&Units=SI |

# 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 |

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