# 7-chloroheptyl dichloroacetate

**Other names:** 1-Heptanol, 7-chloro, dichloroacetate
**Inchi:** InChI=1S/C9H15Cl3O2/c10-6-4-2-1-3-5-7-14-9(13)8(11)12/h8H,1-7H2
**InchiKey:** LUGGQXMJRCRYAK-UHFFFAOYSA-N
**Formula:** C9H15Cl3O2
**SMILES:** O=C(OCCCCCCCCl)C(Cl)Cl
**Mol. weight [g/mol]:** 261.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -247.25 | kJ/mol | Joback Method |
| hf | -526.39 | kJ/mol | Joback Method |
| hfus | 30.92 | kJ/mol | Joback Method |
| hvap | 57.55 | kJ/mol | Joback Method |
| log10ws | -3.52 | | Crippen Method |
| logp | 3.523 | | Crippen Method |
| mcvol | 181.830 | ml/mol | McGowan Method |
| pc | 2185.64 | kPa | Joback Method |
| rinpol | 1654.00 | | NIST Webbook |
| rinpol | 1661.00 | | NIST Webbook |
| rinpol | 1636.00 | | NIST Webbook |
| rinpol | 1646.00 | | NIST Webbook |
| ripol | 2377.00 | | NIST Webbook |
| ripol | 2409.00 | | NIST Webbook |
| ripol | 2395.00 | | NIST Webbook |
| tb | 593.46 | K | Joback Method |
| tc | 785.47 | K | Joback Method |
| tf | 338.11 | K | Joback Method |
| vc | 0.705 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 406.89 | J/mol×K | 593.46 | Joback Method |
| cpg | 418.76 | J/mol×K | 625.46 | Joback Method |

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|---|---|---|---|---|
| cpg | 430.04 | J/mol×K | 657.46 | Joback Method |
| cpg | 440.73 | J/mol×K | 689.46 | Joback Method |
| cpg | 450.85 | J/mol×K | 721.47 | Joback Method |
| cpg | 460.41 | J/mol×K | 753.47 | Joback Method |
| cpg | 469.43 | J/mol×K | 785.47 | Joback Method |
| dvisc | 0.0028129 | Pa×s | 338.11 | Joback Method |
| dvisc | 0.0014150 | Pa×s | 380.67 | Joback Method |
| dvisc | 0.0008173 | Pa×s | 423.23 | Joback Method |
| dvisc | 0.0005219 | Pa×s | 465.79 | Joback Method |
| dvisc | 0.0003592 | Pa×s | 508.34 | Joback Method |
| dvisc | 0.0002619 | Pa×s | 550.90 | Joback Method |
| dvisc | 0.0001999 | Pa×s | 593.46 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R111849&Units=SI
**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

# 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