# Chloromethyl 6-chloro-octanoate

**Other names:** 6-Chlorooctanoic acid, chloromethyl ester
**Inchi:** InChI=1S/C9H16Cl2O2/c1-2-8(11)5-3-4-6-9(12)13-7-10/h8H,2-7H2,1H3
**InchiKey:** XCSMASOBOZXNSF-UHFFFAOYSA-N
**Formula:** C9H16Cl2O2
**SMILES:** CCC(Cl)CCCCC(=O)OCCl
**Mol. weight [g/mol]:** 227.13
**CAS:** 80418-68-4

## 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 | 1481.00 | | NIST Webbook |
| rinpol | 1487.00 | | NIST Webbook |
| rinpol | 1494.00 | | NIST Webbook |
| ripol | 2107.00 | | NIST Webbook |
| ripol | 2075.00 | | NIST Webbook |
| ripol | 2096.00 | | 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 |

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|---|---|---|---|---|
| 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

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C80418684&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