# Chloromethyl octanoate

**Other names:** Octanoic acid, chloromethyl ester
**Inchi:** InChI=1S/C9H17ClO2/c1-2-3-4-5-6-7-9(11)12-8-10/h2-8H2,1H3
**InchiKey:** JRCUJOMLYAQHDP-UHFFFAOYSA-N
**Formula:** C9H17ClO2
**SMILES:** CCCCCCCC(=O)OCCl
**Mol. weight [g/mol]:** 192.68
**CAS:** 61413-70-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -220.95 | kJ/mol | Joback Method |
| hf | -489.63 | kJ/mol | Joback Method |
| hfus | 26.05 | kJ/mol | Joback Method |
| hvap | 49.17 | kJ/mol | Joback Method |
| log10ws | -3.10 | | Crippen Method |
| logp | 3.086 | | Crippen Method |
| mcvol | 157.350 | ml/mol | McGowan Method |
| pc | 2327.03 | kPa | Joback Method |
| rinpol | 1286.00 | | NIST Webbook |
| rinpol | 1263.00 | | NIST Webbook |
| rinpol | 1278.00 | | NIST Webbook |
| ripol | 1684.00 | | NIST Webbook |
| ripol | 1719.00 | | NIST Webbook |
| ripol | 1684.00 | | NIST Webbook |
| ripol | 1700.00 | | NIST Webbook |
| tb | 519.04 | K | Joback Method |
| tc | 698.13 | K | Joback Method |
| tf | 293.27 | K | Joback Method |
| vc | 0.613 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 352.11 | J/mol×K | 519.04 | Joback Method |

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|---|---|---|---|---|
| cpg | 364.91 | J/mol×K | 548.89 | Joback Method |
| cpg | 377.20 | J/mol×K | 578.74 | Joback Method |
| cpg | 388.97 | J/mol×K | 608.58 | Joback Method |
| cpg | 400.25 | J/mol×K | 638.43 | Joback Method |
| cpg | 411.03 | J/mol×K | 668.28 | Joback Method |
| cpg | 421.32 | J/mol×K | 698.13 | Joback Method |
| dvisc | 0.0029830 | Pa×s | 293.27 | Joback Method |
| dvisc | 0.0015445 | Pa×s | 330.90 | Joback Method |
| dvisc | 0.0009148 | Pa×s | 368.53 | Joback Method |
| dvisc | 0.0005970 | Pa×s | 406.15 | Joback Method |
| dvisc | 0.0004189 | Pa×s | 443.78 | Joback Method |
| dvisc | 0.0003106 | Pa×s | 481.41 | Joback Method |
| dvisc | 0.0002406 | Pa×s | 519.04 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C61413705&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