# Propanoic acid, 2-chloro-, 1-methylbutyl ester

**Other names:** 2-Chloropropionic acid, 2-pentyl ester
**Inchi:** InChI=1S/C8H15ClO2/c1-4-5-6(2)11-8(10)7(3)9/h6-7H,4-5H2,1-3H3
**InchiKey:** QTQYTMIPKPUVCH-UHFFFAOYSA-N
**Formula:** C8H15ClO2
**SMILES:** CCCC(C)OC(=O)C(C)Cl
**Mol. weight [g/mol]:** 178.66
**CAS:** 88736-64-5

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -234.25 | kJ/mol | Joback Method |
| hf | -479.55 | kJ/mol | Joback Method |
| hfus | 16.41 | kJ/mol | Joback Method |
| hvap | 46.17 | kJ/mol | Joback Method |
| log10ws | -2.41 | | Crippen Method |
| logp | 2.345 | | Crippen Method |
| mcvol | 143.260 | ml/mol | McGowan Method |
| pc | 2600.43 | kPa | Joback Method |
| rinpol | 1063.00 | | NIST Webbook |
| rinpol | 1050.00 | | NIST Webbook |
| rinpol | 1050.00 | | NIST Webbook |
| rinpol | 1059.00 | | NIST Webbook |
| rinpol | 1067.00 | | NIST Webbook |
| rinpol | 1045.00 | | NIST Webbook |
| ripol | 1389.00 | | NIST Webbook |
| ripol | 1385.00 | | NIST Webbook |
| ripol | 1387.00 | | NIST Webbook |
| ripol | 1404.00 | | NIST Webbook |
| tb | 495.28 | K | Joback Method |
| tc | 683.89 | K | Joback Method |
| tf | 252.00 | K | Joback Method |
| vc | 0.544 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 308.11 | J/mol×K | 495.28 | Joback Method |
| cpg | 320.63 | J/mol×K | 526.72 | Joback Method |
| cpg | 332.62 | J/mol×K | 558.15 | Joback Method |
| cpg | 344.09 | J/mol×K | 589.59 | Joback Method |
| cpg | 355.06 | J/mol×K | 621.02 | Joback Method |
| cpg | 365.51 | J/mol×K | 652.46 | Joback Method |
| cpg | 375.47 | J/mol×K | 683.89 | Joback Method |
| dvisc | 0.0061890 | Pa×s | 252.00 | Joback Method |
| dvisc | 0.0024580 | Pa×s | 292.55 | Joback Method |
| dvisc | 0.0012223 | Pa×s | 333.09 | Joback Method |
| dvisc | 0.0007073 | Pa×s | 373.64 | Joback Method |
| dvisc | 0.0004556 | Pa×s | 414.19 | Joback Method |
| dvisc | 0.0003174 | Pa×s | 454.73 | Joback Method |
| dvisc | 0.0002346 | Pa×s | 495.28 | Joback Method |

# Sources

**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=C88736645&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 |
| **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 |