# Butanoic acid, 2-chloro, 1-methylpropyl ester

**Inchi:** InChI=1S/C8H15ClO2/c1-4-6(3)11-8(10)7(9)5-2/h6-7H,4-5H2,1-3H3
**InchiKey:** HRJQRWBJIJWOEO-UHFFFAOYSA-N
**Formula:** C8H15ClO2
**SMILES:** CCC(C)OC(=O)C(Cl)CC
**Mol. weight [g/mol]:** 178.66

## 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 | 1065.00 | | NIST Webbook |
| rinpol | 1074.00 | | NIST Webbook |
| rinpol | 1050.00 | | NIST Webbook |
| rinpol | 1062.00 | | NIST Webbook |
| rinpol | 1054.00 | | NIST Webbook |
| ripol | 1375.00 | | NIST Webbook |
| ripol | 1380.00 | | NIST Webbook |
| ripol | 1405.00 | | NIST Webbook |
| ripol | 1385.00 | | 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 |

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

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|---|---|
| **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=R28607&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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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