# Butanoic acid, 4-chloro, 1-methylpropyl ester

**Inchi:** InChI=1S/C8H15ClO2/c1-3-7(2)11-8(10)5-4-6-9/h7H,3-6H2,1-2H3
**InchiKey:** MNQRSRRISUUYTQ-UHFFFAOYSA-N
**Formula:** C8H15ClO2
**SMILES:** CCC(C)OC(=O)CCCCl
**Mol. weight [g/mol]:** 178.66

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -231.81 | kJ/mol | Joback Method |
| hf | -474.27 | kJ/mol | Joback Method |
| hfus | 19.94 | kJ/mol | Joback Method |
| hvap | 46.55 | kJ/mol | Joback Method |
| log10ws | -2.30 | | Crippen Method |
| logp | 2.347 | | Crippen Method |
| mcvol | 143.260 | ml/mol | McGowan Method |
| pc | 2579.34 | kPa | Joback Method |
| rinpol | 1154.00 | | NIST Webbook |
| rinpol | 1130.00 | | NIST Webbook |
| rinpol | 1140.00 | | NIST Webbook |
| rinpol | 1134.00 | | NIST Webbook |
| rinpol | 1134.00 | | NIST Webbook |
| rinpol | 1145.00 | | NIST Webbook |
| ripol | 1566.00 | | NIST Webbook |
| ripol | 1539.00 | | NIST Webbook |
| ripol | 1541.00 | | NIST Webbook |
| ripol | 1550.00 | | NIST Webbook |
| tb | 495.72 | K | Joback Method |
| tc | 680.38 | K | Joback Method |
| tf | 267.00 | K | Joback Method |
| vc | 0.550 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

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|---|---|---|---|---|
| cpg | 307.89 | J/mol×K | 495.72 | Joback Method |
| cpg | 320.07 | J/mol×K | 526.50 | Joback Method |
| cpg | 331.75 | J/mol×K | 557.27 | Joback Method |
| cpg | 342.95 | J/mol×K | 588.05 | Joback Method |
| cpg | 353.67 | J/mol×K | 618.82 | Joback Method |
| cpg | 363.91 | J/mol×K | 649.60 | Joback Method |
| cpg | 373.67 | J/mol×K | 680.38 | Joback Method |
| dvisc | 0.0042242 | Pa×s | 267.00 | Joback Method |
| dvisc | 0.0019599 | Pa×s | 305.12 | Joback Method |
| dvisc | 0.0010785 | Pa×s | 343.24 | Joback Method |
| dvisc | 0.0006687 | Pa×s | 381.36 | Joback Method |
| dvisc | 0.0004523 | Pa×s | 419.48 | Joback Method |
| dvisc | 0.0003265 | Pa×s | 457.60 | Joback Method |
| dvisc | 0.0002478 | Pa×s | 495.72 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R28910&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
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# 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 |