# Butanoic acid, 3-chloro, 1-methylethyl ester

**Inchi:** InChI=1S/C7H13ClO2/c1-5(2)10-7(9)4-6(3)8/h5-6H,4H2,1-3H3
**InchiKey:** RRJXSIDJOSFDSU-UHFFFAOYSA-N
**Formula:** C7H13ClO2
**SMILES:** CC(Cl)CC(=O)OC(C)C
**Mol. weight [g/mol]:** 164.63

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -242.67 | kJ/mol | Joback Method |
| hf | -458.91 | kJ/mol | Joback Method |
| hfus | 13.82 | kJ/mol | Joback Method |
| hvap | 43.94 | kJ/mol | Joback Method |
| log10ws | -1.99 | | Crippen Method |
| logp | 1.955 | | Crippen Method |
| mcvol | 129.170 | ml/mol | McGowan Method |
| pc | 2875.03 | kPa | Joback Method |
| rinpol | 982.00 | | NIST Webbook |
| rinpol | 974.00 | | NIST Webbook |
| rinpol | 968.00 | | NIST Webbook |
| rinpol | 990.00 | | NIST Webbook |
| rinpol | 988.00 | | NIST Webbook |
| ripol | 1356.00 | | NIST Webbook |
| ripol | 1347.00 | | NIST Webbook |
| ripol | 1353.00 | | NIST Webbook |
| ripol | 1376.00 | | NIST Webbook |
| ripol | 1356.00 | | NIST Webbook |
| tb | 472.40 | K | Joback Method |
| tc | 663.16 | K | Joback Method |
| tf | 240.73 | K | Joback Method |
| vc | 0.488 | m3/kmol | Joback Method |

## Temperature Dependent Properties

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

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|---|---|---|---|---|
| cpg | 265.59 | J/mol×K | 472.40 | Joback Method |
| cpg | 277.03 | J/mol×K | 504.19 | Joback Method |
| cpg | 288.00 | J/mol×K | 535.99 | Joback Method |
| cpg | 298.52 | J/mol×K | 567.78 | Joback Method |
| cpg | 308.57 | J/mol×K | 599.57 | Joback Method |
| cpg | 318.17 | J/mol×K | 631.37 | Joback Method |
| cpg | 327.32 | J/mol×K | 663.16 | Joback Method |
| dvisc | 0.0064287 | Pa×s | 240.73 | Joback Method |
| dvisc | 0.0025878 | Pa×s | 279.34 | Joback Method |
| dvisc | 0.0012993 | Pa×s | 317.95 | Joback Method |
| dvisc | 0.0007574 | Pa×s | 356.56 | Joback Method |
| dvisc | 0.0004906 | Pa×s | 395.18 | Joback Method |
| dvisc | 0.0003433 | Pa×s | 433.79 | Joback Method |
| dvisc | 0.0002547 | Pa×s | 472.40 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R28750&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 |