# Butanoic acid, 4-chloro, 2-propenyl ester

**Inchi:** InChI=1S/C7H11ClO2/c1-2-6-10-7(9)4-3-5-8/h2H,1,3-6H2
**InchiKey:** NSCJTNOFIYBWFN-UHFFFAOYSA-N
**Formula:** C7H11ClO2
**SMILES:** C=CCOC(=O)CCCCl
**Mol. weight [g/mol]:** 162.61

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -149.95 | kJ/mol | Joback Method |
| hf | -322.92 | kJ/mol | Joback Method |
| hfus | 19.59 | kJ/mol | Joback Method |
| hvap | 44.05 | kJ/mol | Joback Method |
| log10ws | -1.62 | | Crippen Method |
| logp | 1.735 | | Crippen Method |
| mcvol | 124.870 | ml/mol | McGowan Method |
| pc | 2956.90 | kPa | Joback Method |
| rinpol | 1097.00 | | NIST Webbook |
| rinpol | 1097.00 | | NIST Webbook |
| rinpol | 1077.00 | | NIST Webbook |
| rinpol | 1105.00 | | NIST Webbook |
| ripol | 1692.00 | | NIST Webbook |
| ripol | 1671.00 | | NIST Webbook |
| tb | 469.96 | K | Joback Method |
| tc | 656.31 | K | Joback Method |
| tf | 268.97 | K | Joback Method |
| vc | 0.481 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 248.36 | J/mol×K | 469.96 | Joback Method |
| cpg | 258.49 | J/mol×K | 501.02 | Joback Method |
| cpg | 268.20 | J/mol×K | 532.08 | Joback Method |
| cpg | 277.49 | J/mol×K | 563.14 | Joback Method |

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|---|---|---|---|---|
| cpg | 286.38 | J/mol×K | 594.19 | Joback Method |
| cpg | 294.86 | J/mol×K | 625.25 | Joback Method |
| cpg | 302.94 | J/mol×K | 656.31 | Joback Method |
| dvisc | 0.0028258 | Pa×s | 268.97 | Joback Method |
| dvisc | 0.0015592 | Pa×s | 302.47 | Joback Method |
| dvisc | 0.0009687 | Pa×s | 335.97 | Joback Method |
| dvisc | 0.0006561 | Pa×s | 369.47 | Joback Method |
| dvisc | 0.0004741 | Pa×s | 402.96 | Joback Method |
| dvisc | 0.0003601 | Pa×s | 436.46 | Joback Method |
| dvisc | 0.0002844 | Pa×s | 469.96 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R28938&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