# Butanoic acid, 3-chloroprop-2-enyl ester

**Inchi:** InChI=1S/C7H11ClO2/c1-2-4-7(9)10-6-3-5-8/h3,5H,2,4,6H2,1H3/b5-3+
**InchiKey:** RVCJBAWEOOBVCN-HWKANZROSA-N
**Formula:** C7H11ClO2
**SMILES:** CCCC(=O)OCC=CCl
**Mol. weight [g/mol]:** 162.61

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -157.57 | kJ/mol | Joback Method |
| hf | -331.13 | kJ/mol | Joback Method |
| hfus | 21.07 | kJ/mol | Joback Method |
| hvap | 44.67 | kJ/mol | Joback Method |
| log10ws | -2.12 | | Crippen Method |
| logp | 2.082 | | Crippen Method |
| mcvol | 124.870 | ml/mol | McGowan Method |
| pc | 2989.32 | kPa | Joback Method |
| tb | 477.44 | K | Joback Method |
| tc | 668.66 | K | Joback Method |
| tf | 265.65 | K | Joback Method |
| vc | 0.480 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 248.14 | J/mol×K | 477.44 | Joback Method |
| cpg | 295.25 | J/mol×K | 636.79 | Joback Method |
| cpg | 286.73 | J/mol×K | 604.92 | Joback Method |
| cpg | 277.76 | J/mol×K | 573.05 | Joback Method |
| cpg | 268.35 | J/mol×K | 541.18 | Joback Method |
| cpg | 258.48 | J/mol×K | 509.31 | Joback Method |
| cpg | 303.36 | J/mol×K | 668.66 | Joback Method |
| dvisc | 0.0002365 | Pa×s | 477.44 | Joback Method |
| dvisc | 0.0003032 | Pa×s | 442.14 | Joback Method |
| dvisc | 0.0004058 | Pa×s | 406.84 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0005741 | Pa×s | 371.54 | Joback Method |
| dvisc | 0.0008735 | Pa×s | 336.25 | Joback Method |
| dvisc | 0.0014665 | Pa×s | 300.95 | Joback Method |
| dvisc | 0.0028256 | Pa×s | 265.65 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U299127&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
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume