# Butanoic acid, 4-chloro-3-oxo-, ethyl ester

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|---|---|
| **Other names:** | Ethyl 4-chloroacetoacetate |
| | Ethyl «gamma»-chloroacetoacetate |
| | 4-Chloroacetoacetic acid ethyl ester |
| | Acetoacetic acid, 4-chloro-, ethyl ester |
| **Inchi:** | InChI=1S/C6H9ClO3/c1-2-10-6(9)3-5(8)4-7/h2-4H2,1H3 |
| **InchiKey:** | OHLRLMWUFVDREV-UHFFFAOYSA-N |
| **Formula:** | C6H9ClO3 |
| **SMILES:** | CCOC(=O)CC(=O)CCl |
| **Mol. weight [g/mol]:** | 164.59 |
| **CAS:** | 638-07-3 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -375.13 | kJ/mol | Joback Method |
| hf | -540.29 | kJ/mol | Joback Method |
| hfus | 19.88 | kJ/mol | Joback Method |
| hvap | 49.24 | kJ/mol | Joback Method |
| log10ws | -0.63 | | Crippen Method |
| logp | 0.747 | | Crippen Method |
| mcvol | 116.650 | ml/mol | McGowan Method |
| pc | 3372.36 | kPa | Joback Method |
| tb | 504.27 | K | Joback Method |
| tc | 698.73 | K | Joback Method |
| tf | 309.39 | K | Joback Method |
| vc | 0.451 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 238.35 | J/mol×K | 504.27 | Joback Method |
| cpg | 247.32 | J/mol×K | 536.68 | Joback Method |
| cpg | 255.91 | J/mol×K | 569.09 | Joback Method |
| cpg | 264.12 | J/mol×K | 601.50 | Joback Method |
| cpg | 271.94 | J/mol×K | 633.91 | Joback Method |

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|---|---|---|---|---|
| cpg | 279.39 | J/mol×K | 666.32 | Joback Method |
| cpg | 286.45 | J/mol×K | 698.73 | Joback Method |
| dvisc | 0.0026181 | Pa×s | 309.39 | Joback Method |
| dvisc | 0.0015720 | Pa×s | 341.87 | Joback Method |
| dvisc | 0.0010312 | Pa×s | 374.35 | Joback Method |
| dvisc | 0.0007236 | Pa×s | 406.83 | Joback Method |
| dvisc | 0.0005350 | Pa×s | 439.31 | Joback Method |
| dvisc | 0.0004124 | Pa×s | 471.79 | Joback Method |
| dvisc | 0.0003287 | Pa×s | 504.27 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 388.20 | K | 1.90 | NIST Webbook |

# Sources

**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=C638073&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

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|---|---|
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |