# Hexyl 4-chlorobutanoate

**Other names:** Butanoic acid, 4-chloro, hexyl ester
**Inchi:** InChI=1S/C10H19ClO2/c1-2-3-4-5-9-13-10(12)7-6-8-11/h2-9H2,1H3
**InchiKey:** NJJCFVMCDUBLGH-UHFFFAOYSA-N
**Formula:** C10H19ClO2
**SMILES:** CCCCCCOC(=O)CCCCl
**Mol. weight [g/mol]:** 206.71

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -212.53 | kJ/mol | Joback Method |
| hf | -510.27 | kJ/mol | Joback Method |
| hfus | 28.64 | kJ/mol | Joback Method |
| hvap | 51.39 | kJ/mol | Joback Method |
| log10ws | -3.02 | | Crippen Method |
| logp | 3.129 | | Crippen Method |
| mcvol | 171.440 | ml/mol | McGowan Method |
| pc | 2125.60 | kPa | Joback Method |
| rinpol | 1418.00 | | NIST Webbook |
| rinpol | 1417.00 | | NIST Webbook |
| rinpol | 1409.00 | | NIST Webbook |
| rinpol | 1401.00 | | NIST Webbook |
| rinpol | 1401.00 | | NIST Webbook |
| rinpol | 1401.00 | | NIST Webbook |
| rinpol | 1409.00 | | NIST Webbook |
| rinpol | 1417.00 | | NIST Webbook |
| tb | 541.92 | K | Joback Method |
| tc | 719.34 | K | Joback Method |
| tf | 304.54 | K | Joback Method |
| vc | 0.668 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 398.46 | J/mol×K | 541.92 | Joback Method |

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|---|---|---|---|---|
| cpg | 461.13 | J/mol×K | 689.77 | Joback Method |
| cpg | 449.68 | J/mol×K | 660.20 | Joback Method |
| cpg | 437.70 | J/mol×K | 630.63 | Joback Method |
| cpg | 425.18 | J/mol×K | 601.06 | Joback Method |
| cpg | 412.10 | J/mol×K | 571.49 | Joback Method |
| cpg | 472.05 | J/mol×K | 719.34 | Joback Method |
| dvisc | 0.0002192 | Pa×s | 541.92 | Joback Method |
| dvisc | 0.0002844 | Pa×s | 502.36 | Joback Method |
| dvisc | 0.0003858 | Pa×s | 462.79 | Joback Method |
| dvisc | 0.0005540 | Pa×s | 423.23 | Joback Method |
| dvisc | 0.0008572 | Pa×s | 383.67 | Joback Method |
| dvisc | 0.0014664 | Pa×s | 344.10 | Joback Method |
| dvisc | 0.0028840 | Pa×s | 304.54 | Joback Method |

# Sources

**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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R28287&Units=SI

# 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

**tb:** Normal Boiling Point Temperature

**tc:** Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume