# Propyl 4-chlorobutanoate

**Other names:** Propyl 4-chlorobutanoate
n-Propyl-4-chlorobutyrate
**Inchi:** InChI=1S/C7H13ClO2/c1-2-6-10-7(9)4-3-5-8/h2-6H2,1H3
**InchiKey:** RGFHUYWGQUDWDL-UHFFFAOYSA-N
**Formula:** C7H13ClO2
**SMILES:** CCCOC(=O)CCCCl
**Mol. weight [g/mol]:** 164.63

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.5397 | | Cheméo Relay (1.0) |
| chl | -4044.70 ± 8.40 | kJ/mol | NIST Webbook |
| chl | -4037.00 | kJ/mol | NIST Webbook |
| hf | -538.10 ± 9.60 | kJ/mol | NIST Webbook |
| hfl | -591.60 ± 8.40 | kJ/mol | NIST Webbook |
| hfus | 20.87 | kJ/mol | Joback Method |
| hvap | 53.60 ± 4.20 | kJ/mol | NIST Webbook |
| ie | 10.15 | eV | Cheméo Relay (1.0) |
| log10ws | -1.82 | | Cheméo Relay (1.0) |
| logp | 1.959 | | Crippen Method |
| mcvol | 129.170 | ml/mol | McGowan Method |
| pc | 2826.33 | kPa | Joback Method |
| rinpol | 1117.00 | | NIST Webbook |
| rinpol | 1110.00 | | NIST Webbook |
| rinpol | 1100.00 | | NIST Webbook |
| rinpol | 1102.00 | | NIST Webbook |
| rinpol | 1117.00 | | NIST Webbook |
| tb | 463.41 | K | Cheméo Relay (1.0) |
| tc | 646.63 | K | Cheméo Relay (1.0) |
| tf | 207.26 | K | Cheméo Relay (1.0) |
| vc | 0.480 | m3/kmol | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 265.22 | J/mol×K | 473.28 | Joback Method |
| cpg | 276.01 | J/mol×K | 503.72 | Joback Method |
| cpg | 286.40 | J/mol×K | 534.15 | Joback Method |
| cpg | 296.38 | J/mol×K | 564.59 | Joback Method |
| cpg | 305.96 | J/mol×K | 595.03 | Joback Method |
| cpg | 315.13 | J/mol×K | 625.46 | Joback Method |
| cpg | 323.90 | J/mol×K | 655.90 | Joback Method |
| dvisc | 0.0030645 | Pa×s | 270.73 | Joback Method |
| dvisc | 0.0016518 | Pa×s | 304.49 | Joback Method |
| dvisc | 0.0010072 | Pa×s | 338.25 | Joback Method |
| dvisc | 0.0006719 | Pa×s | 372.00 | Joback Method |
| dvisc | 0.0004794 | Pa×s | 405.76 | Joback Method |
| dvisc | 0.0003603 | Pa×s | 439.52 | Joback Method |
| dvisc | 0.0002820 | Pa×s | 473.28 | Joback Method |

# Sources

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C3153353&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# Legend

**af:** Acentric Factor

**chl:** Standard liquid enthalpy of combustion

**cpg:** Ideal gas heat capacity

**dvisc:** Dynamic viscosity

**hf:** Enthalpy of formation at standard conditions

**hfl:** Liquid phase enthalpy of formation at standard conditions

**hfus:** Enthalpy of fusion at standard conditions

**hvap:** Enthalpy of vaporization at standard conditions

**ie:** Ionization energy

**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 |