# Propanoic acid, 3-chloro-, propyl ester

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|---|---|
| **Other names:** | propyl 3-chloropropionate |
| | n-Propyl-3-chloropropionate |
| **Inchi:** | InChI=1S/C6H11ClO2/c1-2-5-9-6(8)3-4-7/h2-5H2,1H3 |
| **InchiKey:** | WIOAODPBBXZVNV-UHFFFAOYSA-N |
| **Formula:** | C6H11ClO2 |
| **SMILES:** | CCCOC(=O)CCCl |
| **Mol. weight [g/mol]:** | 150.60 |
| **CAS:** | 62108-66-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -3413.00 | kJ/mol | NIST Webbook |
| chl | -3479.00 ± 4.00 | kJ/mol | NIST Webbook |
| chl | -3419.20 ± 8.40 | kJ/mol | NIST Webbook |
| gf | -246.21 | kJ/mol | Joback Method |
| hf | -485.80 ± 9.60 | kJ/mol | NIST Webbook |
| hfl | -537.60 ± 8.40 | kJ/mol | NIST Webbook |
| hfus | 18.28 | kJ/mol | Joback Method |
| hvap | 51.90 ± 4.20 | kJ/mol | NIST Webbook |
| log10ws | -1.35 | | Crippen Method |
| logp | 1.568 | | Crippen Method |
| mcvol | 115.080 | ml/mol | McGowan Method |
| pc | 3138.51 | kPa | Joback Method |
| rinpol | 985.00 | | NIST Webbook |
| rinpol | 998.00 | | NIST Webbook |
| rinpol | 1000.00 | | NIST Webbook |
| rinpol | 1003.00 | | NIST Webbook |
| rinpol | 986.00 | | NIST Webbook |
| rinpol | 996.00 | | NIST Webbook |
| rinpol | 978.00 | | NIST Webbook |
| rinpol | 996.00 | | NIST Webbook |
| ripol | 1488.00 | | NIST Webbook |
| ripol | 1497.00 | | NIST Webbook |
| ripol | 1470.00 | | NIST Webbook |
| ripol | 1454.00 | | NIST Webbook |
| ripol | 1464.00 | | NIST Webbook |
| ripol | 1450.00 | | NIST Webbook |

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|---|---|---|---|
| ripol | 1469.00 | | NIST Webbook |
| ripol | 1489.00 | | NIST Webbook |
| tb | 450.40 | K | Joback Method |
| tc | 634.77 | K | Joback Method |
| tf | 259.46 | K | Joback Method |
| vc | 0.445 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 224.90 | J/mol×K | 450.40 | Joback Method |
| cpg | 234.51 | J/mol×K | 481.13 | Joback Method |
| cpg | 243.77 | J/mol×K | 511.86 | Joback Method |
| cpg | 252.68 | J/mol×K | 542.58 | Joback Method |
| cpg | 261.25 | J/mol×K | 573.31 | Joback Method |
| cpg | 269.47 | J/mol×K | 604.04 | Joback Method |
| cpg | 277.34 | J/mol×K | 634.77 | Joback Method |
| dvisc | 0.0030315 | Pa×s | 259.46 | Joback Method |
| dvisc | 0.0016707 | Pa×s | 291.28 | Joback Method |
| dvisc | 0.0010354 | Pa×s | 323.11 | Joback Method |
| dvisc | 0.0006992 | Pa×s | 354.93 | Joback Method |
| dvisc | 0.0005036 | Pa×s | 386.75 | Joback Method |
| dvisc | 0.0003813 | Pa×s | 418.58 | Joback Method |
| dvisc | 0.0003003 | Pa×s | 450.40 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C62108661&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

**chl:** Standard liquid enthalpy of combustion

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **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 |
| **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 |