# Propanoyl chloride

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|---|---|
| **Other names:** | Propionyl chloride |
| | Propionic chloride |
| | Propionic acid chloride |
| | UN 1815 |
| **Inchi:** | InChI=1S/C3H5ClO/c1-2-3(4)5/h2H2,1H3 |
| **InchiKey:** | RZWZRACFZGVKFM-UHFFFAOYSA-N |
| **Formula:** | C3H5ClO |
| **SMILES:** | CCC(=O)Cl |
| **Mol. weight [g/mol]:** | 92.52 |
| **CAS:** | 79-03-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -166.47 | kJ/mol | Joback Method |
| hf | -233.57 | kJ/mol | Joback Method |
| hfus | 9.32 | kJ/mol | Joback Method |
| hvap | 33.40 | kJ/mol | Joback Method |
| log10ws | -1.01 | | Crippen Method |
| logp | 1.162 | | Crippen Method |
| mcvol | 66.940 | ml/mol | McGowan Method |
| pc | 4565.38 | kPa | Joback Method |
| rinpol | 626.00 | | NIST Webbook |
| tb | 359.34 | K | Joback Method |
| tc | 547.77 | K | Joback Method |
| tf | 179.20 ± 0.40 | K | NIST Webbook |
| vc | 0.259 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 128.69 | J/mol×K | 547.77 | Joback Method |
| cpg | 124.35 | J/mol×K | 516.37 | Joback Method |
| cpg | 119.80 | J/mol×K | 484.96 | Joback Method |
| cpg | 115.05 | J/mol×K | 453.56 | Joback Method |

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|---|---|---|---|---|
| cpg | 110.08 | J/mol×K | 422.15 | Joback Method |
| cpg | 104.90 | J/mol×K | 390.75 | Joback Method |
| cpg | 99.49 | J/mol×K | 359.34 | Joback Method |
| cpl | 147.30 | J/mol×K | 298.00 | NIST Webbook |
| dvisc | 0.0004415 | Pa×s | 333.35 | Joback Method |
| dvisc | 0.0005704 | Pa×s | 307.37 | Joback Method |
| dvisc | 0.0007728 | Pa×s | 281.38 | Joback Method |
| dvisc | 0.0011136 | Pa×s | 255.39 | Joback Method |
| dvisc | 0.0017433 | Pa×s | 229.41 | Joback Method |
| dvisc | 0.0030601 | Pa×s | 203.42 | Joback Method |
| dvisc | 0.0003546 | Pa×s | 359.34 | Joback Method |

# Sources

**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=C79038&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# Legend

**cpg:** Ideal gas heat capacity
**cpl:** Liquid phase 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