# Heptanoic acid, 7-chloro, ethyl ester

**Inchi:** InChI=1S/C9H17ClO2/c1-2-12-9(11)7-5-3-4-6-8-10/h2-8H2,1H3
**InchiKey:** MTVFBQCYLUWYAS-UHFFFAOYSA-N
**Formula:** C9H17ClO2
**SMILES:** CCOC(=O)CCCCCCCl
**Mol. weight [g/mol]:** 192.68

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -220.95 | kJ/mol | Joback Method |
| hf | -489.63 | kJ/mol | Joback Method |
| hfus | 26.05 | kJ/mol | Joback Method |
| hvap | 49.17 | kJ/mol | Joback Method |
| log10ws | -2.61 | | Crippen Method |
| logp | 2.739 | | Crippen Method |
| mcvol | 157.350 | ml/mol | McGowan Method |
| pc | 2327.03 | kPa | Joback Method |
| rinpol | 1339.00 | | NIST Webbook |
| ripol | 1880.00 | | NIST Webbook |
| ripol | 1880.00 | | NIST Webbook |
| tb | 519.04 | K | Joback Method |
| tc | 698.13 | K | Joback Method |
| tf | 293.27 | K | Joback Method |
| vc | 0.613 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 352.11 | J/mol×K | 519.04 | Joback Method |
| cpg | 364.91 | J/mol×K | 548.89 | Joback Method |
| cpg | 377.20 | J/mol×K | 578.74 | Joback Method |
| cpg | 388.97 | J/mol×K | 608.58 | Joback Method |
| cpg | 400.25 | J/mol×K | 638.43 | Joback Method |
| cpg | 411.03 | J/mol×K | 668.28 | Joback Method |
| cpg | 421.32 | J/mol×K | 698.13 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0029830 | Pa×s | 293.27 | Joback Method |
| dvisc | 0.0015445 | Pa×s | 330.90 | Joback Method |
| dvisc | 0.0009148 | Pa×s | 368.53 | Joback Method |
| dvisc | 0.0005970 | Pa×s | 406.15 | Joback Method |
| dvisc | 0.0004189 | Pa×s | 443.78 | Joback Method |
| dvisc | 0.0003106 | Pa×s | 481.41 | Joback Method |
| dvisc | 0.0002406 | Pa×s | 519.04 | Joback Method |

# Sources

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|---|---|
| **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=R91785&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 |
| **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 |

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