# Heptanoic acid, 2-iodoethyl ester

**Inchi:** InChI=1S/C9H17IO2/c1-2-3-4-5-6-9(11)12-8-7-10/h2-8H2,1H3
**InchiKey:** LUISAYURPQPDIY-UHFFFAOYSA-N
**Formula:** C9H17IO2
**SMILES:** CCCCCCC(=O)OCCI
**Mol. weight [g/mol]:** 284.13

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -150.90 | kJ/mol | Joback Method |
| hf | -397.02 | kJ/mol | Joback Method |
| hfus | 26.26 | kJ/mol | Joback Method |
| hvap | 54.16 | kJ/mol | Joback Method |
| log10ws | -3.40 | | Crippen Method |
| logp | 2.935 | | Crippen Method |
| mcvol | 170.930 | ml/mol | McGowan Method |
| pc | 2361.07 | kPa | Joback Method |
| rinpol | 1484.00 | | NIST Webbook |
| rinpol | 1484.00 | | NIST Webbook |
| tb | 574.75 | K | Joback Method |
| tc | 775.16 | K | Joback Method |
| tf | 321.41 | K | Joback Method |
| vc | 0.651 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 378.61 | J/mol×K | 574.75 | Joback Method |
| cpg | 437.23 | J/mol×K | 741.76 | Joback Method |
| cpg | 426.72 | J/mol×K | 708.36 | Joback Method |
| cpg | 415.62 | J/mol×K | 674.96 | Joback Method |
| cpg | 403.91 | J/mol×K | 641.55 | Joback Method |
| cpg | 391.58 | J/mol×K | 608.15 | Joback Method |
| cpg | 447.17 | J/mol×K | 775.16 | Joback Method |
| dvisc | 0.0002362 | Pa×s | 574.75 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003062 | Pa×s | 532.53 | Joback Method |
| dvisc | 0.0004151 | Pa×s | 490.30 | Joback Method |
| dvisc | 0.0005960 | Pa×s | 448.08 | Joback Method |
| dvisc | 0.0009225 | Pa×s | 405.86 | Joback Method |
| dvisc | 0.0015803 | Pa×s | 363.63 | Joback Method |
| dvisc | 0.0031185 | Pa×s | 321.41 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R19911&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

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|---|---|
| **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 |