# Ethyl perfluorohexanoate

**Other names:** 2,2,3,3,4,4,5,5,6,6,6-Undecafluoro- hexanoic acid ethyl ester
**Inchi:** InChI=1S/C8H5F11O2/c1-2-21-3(20)4(9,10)5(11,12)6(13,14)7(15,16)8(17,18)19/h2H2,1H
**InchiKey:** PIGASTCSFHUJBM-UHFFFAOYSA-N
**Formula:** C8H5F11O2
**SMILES:** CCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
**Mol. weight [g/mol]:** 342.11

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -2346.15 | kJ/mol | Joback Method |
| hf | -2654.21 | kJ/mol | Joback Method |
| hfus | 16.07 | kJ/mol | Joback Method |
| hvap | 27.09 | kJ/mol | Joback Method |
| log10ws | -3.95 | | Crippen Method |
| logp | 3.653 | | Crippen Method |
| mcvol | 150.490 | ml/mol | McGowan Method |
| pc | 1826.28 | kPa | Joback Method |
| rinpol | 666.00 | | NIST Webbook |
| rinpol | 666.40 | | NIST Webbook |
| tb | 434.55 | K | Joback Method |
| tc | 572.05 | K | Joback Method |
| tf | 270.67 | K | Joback Method |
| vc | 0.650 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 381.88 | J/mol×K | 434.55 | Joback Method |
| cpg | 393.71 | J/mol×K | 457.47 | Joback Method |
| cpg | 404.79 | J/mol×K | 480.38 | Joback Method |
| cpg | 415.15 | J/mol×K | 503.30 | Joback Method |
| cpg | 424.83 | J/mol×K | 526.22 | Joback Method |
| cpg | 433.85 | J/mol×K | 549.13 | Joback Method |
| cpg | 442.24 | J/mol×K | 572.05 | Joback Method |

# Sources

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|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R70094&Units=SI |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |