# Pentafluoropropanamide, N-hexyl-

**Inchi:** InChI=1S/C9H14F5NO/c1-2-3-4-5-6-15-7(16)8(10,11)9(12,13)14/h2-6H2,1H3,(H,15,16)
**InchiKey:** WMVFFBSJXLBQIO-UHFFFAOYSA-N
**Formula:** C9H14F5NO
**SMILES:** CCCCCCNC(=O)C(F)(F)C(F)(F)F
**Mol. weight [g/mol]:** 247.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -983.00 | kJ/mol | Joback Method |
| hf | -1286.25 | kJ/mol | Joback Method |
| hfus | 26.34 | kJ/mol | Joback Method |
| hvap | 42.13 | kJ/mol | Joback Method |
| log10ws | -3.53 | | Crippen Method |
| logp | 2.880 | | Crippen Method |
| mcvol | 158.070 | ml/mol | McGowan Method |
| pc | 2079.33 | kPa | Joback Method |
| rinpol | 1084.00 | | NIST Webbook |
| rinpol | 1084.00 | | NIST Webbook |
| tb | 499.25 | K | Joback Method |
| tc | 656.56 | K | Joback Method |
| tf | 301.57 | K | Joback Method |
| vc | 0.648 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 394.12 | J/mol×K | 499.25 | Joback Method |
| cpg | 406.85 | J/mol×K | 525.47 | Joback Method |
| cpg | 418.90 | J/mol×K | 551.69 | Joback Method |
| cpg | 430.29 | J/mol×K | 577.91 | Joback Method |
| cpg | 441.06 | J/mol×K | 604.12 | Joback Method |
| cpg | 451.23 | J/mol×K | 630.34 | Joback Method |
| cpg | 460.84 | J/mol×K | 656.56 | Joback Method |

# Sources

| | |
|---|---|
| **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=U407335&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 |