# l-Methionine, n-pentafluoropropionyl-, isohexyl ester

**Inchi:** InChI=1S/C14H22F5NO3S/c1-9(2)5-4-7-23-11(21)10(6-8-24-3)20-12(22)13(15,16)14(17

**InchiKey:** ZGCRHFLMSIWKGO-UHFFFAOYSA-N

**Formula:** C14H22F5NO3S

**SMILES:** CSCCC(NC(=O)C(F)(F)C(F)(F)F)C(=O)OCCCC(C)C

**Mol. weight [g/mol]:** 379.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1146.58 | kJ/mol | Joback Method |
| hf | -1602.94 | kJ/mol | Joback Method |
| hfus | 39.16 | kJ/mol | Joback Method |
| hvap | 68.46 | kJ/mol | Joback Method |
| log10ws | -4.24 | | Crippen Method |
| logp | 3.401 | | Crippen Method |
| mcvol | 252.310 | ml/mol | McGowan Method |
| pc | 1486.14 | kPa | Joback Method |
| rinpol | 1750.00 | | NIST Webbook |
| rinpol | 1750.00 | | NIST Webbook |
| tb | 757.84 | K | Joback Method |
| tc | 941.71 | K | Joback Method |
| tf | 434.48 | K | Joback Method |
| vc | 0.995 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 756.63 | J/mol×K | 757.84 | Joback Method |
| cpg | 770.08 | J/mol×K | 788.48 | Joback Method |
| cpg | 782.65 | J/mol×K | 819.13 | Joback Method |
| cpg | 794.37 | J/mol×K | 849.77 | Joback Method |
| cpg | 805.29 | J/mol×K | 880.42 | Joback Method |
| cpg | 815.45 | J/mol×K | 911.06 | Joback Method |
| cpg | 824.88 | J/mol×K | 941.71 | Joback Method |

# Sources

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|---|---|
| **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=U320913&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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