# Leucine-methionine, N(«alpha»,«epsilon»)-trifluoroacetyl-N-O-permeth derivative

**Inchi:** InChI=1S/C16H27F3N2O4S/c1-10(2)9-12(21(4)15(24)16(17,18)19)13(22)20(3)11(7-8-26
**InchiKey:** KIKPQWCEMUACBF-UHFFFAOYSA-N
**Formula:** C16H27F3N2O4S
**SMILES:** COC(=O)C(CCSC)N(C)C(=O)C(CC(C)C)N(C)C(=O)C(F)(F)F
**Mol. weight [g/mol]:** 400.46

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -742.15 | kJ/mol | Joback Method |
| hf | -1279.52 | kJ/mol | Joback Method |
| hfus | 44.61 | kJ/mol | Joback Method |
| hvap | 79.85 | kJ/mol | Joback Method |
| log10ws | -2.60 | | Crippen Method |
| logp | 2.175 | | Crippen Method |
| mcvol | 288.500 | ml/mol | McGowan Method |
| pc | 1412.25 | kPa | Joback Method |
| rinpol | 2054.00 | | NIST Webbook |
| rinpol | 2005.00 | | NIST Webbook |
| rinpol | 2005.00 | | NIST Webbook |
| tb | 836.43 | K | Joback Method |
| tc | 1031.22 | K | Joback Method |
| tf | 500.63 | K | Joback Method |
| vc | 1.083 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 896.06 | J/mol×K | 836.43 | Joback Method |
| cpg | 910.21 | J/mol×K | 868.90 | Joback Method |
| cpg | 923.31 | J/mol×K | 901.36 | Joback Method |
| cpg | 935.44 | J/mol×K | 933.83 | Joback Method |
| cpg | 946.62 | J/mol×K | 966.29 | Joback Method |
| cpg | 956.91 | J/mol×K | 998.76 | Joback Method |
| cpg | 966.35 | J/mol×K | 1031.22 | 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=R248758&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 |