# Sarcosine, n-pentafluorobenzoyl-, hexyl ester

**Inchi:** InChI=1S/C16H18F5NO3/c1-3-4-5-6-7-25-9(23)8-22(2)16(24)10-11(17)13(19)15(21)14(2
**InchiKey:** CSRIUXJUHKNQST-UHFFFAOYSA-N
**Formula:** C16H18F5NO3
**SMILES:** CCCCCCOC(=O)CN(C)C(=O)c1c(F)c(F)c(F)c(F)c1F
**Mol. weight [g/mol]:** 367.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1078.01 | kJ/mol | Joback Method |
| hf | -1464.79 | kJ/mol | Joback Method |
| hfus | 52.10 | kJ/mol | Joback Method |
| hvap | 70.66 | kJ/mol | Joback Method |
| log10ws | -5.07 | | Crippen Method |
| logp | 3.578 | | Crippen Method |
| mcvol | 240.380 | ml/mol | McGowan Method |
| pc | 1461.25 | kPa | Joback Method |
| rinpol | 1966.00 | | NIST Webbook |
| tb | 756.01 | K | Joback Method |
| tc | 934.82 | K | Joback Method |
| tf | 516.61 | K | Joback Method |
| vc | 0.962 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 696.44 | J/mol×K | 756.01 | Joback Method |
| cpg | 709.35 | J/mol×K | 785.81 | Joback Method |
| cpg | 721.51 | J/mol×K | 815.61 | Joback Method |
| cpg | 732.94 | J/mol×K | 845.41 | Joback Method |
| cpg | 743.66 | J/mol×K | 875.22 | Joback Method |
| cpg | 753.66 | J/mol×K | 905.02 | Joback Method |
| cpg | 762.97 | J/mol×K | 934.82 | 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=U321547&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 |
| **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 |