# Sarcosine, n-pentafluorobenzoyl-, ethyl ester

**Inchi:** InChI=1S/C12H10F5NO3/c1-3-21-5(19)4-18(2)12(20)6-7(13)9(15)11(17)10(16)8(6)14/h3
**InchiKey:** CIUFHJXMOVARRA-UHFFFAOYSA-N
**Formula:** C12H10F5NO3
**SMILES:** CCOC(=O)CN(C)C(=O)c1c(F)c(F)c(F)c(F)c1F
**Mol. weight [g/mol]:** 311.20

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1111.69 | kJ/mol | Joback Method |
| hf | -1382.23 | kJ/mol | Joback Method |
| hfus | 41.74 | kJ/mol | Joback Method |
| hvap | 61.75 | kJ/mol | Joback Method |
| log10ws | -3.39 | | Crippen Method |
| logp | 2.017 | | Crippen Method |
| mcvol | 184.020 | ml/mol | McGowan Method |
| pc | 2007.30 | kPa | Joback Method |
| rinpol | 1594.00 | | NIST Webbook |
| rinpol | 1594.00 | | NIST Webbook |
| tb | 664.49 | K | Joback Method |
| tc | 841.75 | K | Joback Method |
| tf | 471.53 | K | Joback Method |
| vc | 0.738 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 485.30 | J/mol×K | 664.49 | Joback Method |
| cpg | 495.99 | J/mol×K | 694.03 | Joback Method |
| cpg | 506.12 | J/mol×K | 723.58 | Joback Method |
| cpg | 515.69 | J/mol×K | 753.12 | Joback Method |
| cpg | 524.71 | J/mol×K | 782.66 | Joback Method |
| cpg | 533.20 | J/mol×K | 812.21 | Joback Method |
| cpg | 541.13 | J/mol×K | 841.75 | Joback Method |

# Sources

| | |
|---|---|
| **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=U321542&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 |