# Sarcosine, N-(2,3,4-trifluorobenzoyl)-, isohexyl ester

**Inchi:** InChI=1S/C16H20F3NO3/c1-10(2)5-4-8-23-13(21)9-20(3)16(22)11-6-7-12(17)15(19)14(1

**InchiKey:** ZHIGJQSJWMSFAF-UHFFFAOYSA-N

**Formula:** C16H20F3NO3

**SMILES:** CC(C)CCCOC(=O)CN(C)C(=O)c1ccc(F)c(F)c1F

**Mol. weight [g/mol]:** 331.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -671.57 | kJ/mol | Joback Method |
| hf | -1054.91 | kJ/mol | Joback Method |
| hfus | 43.19 | kJ/mol | Joback Method |
| hvap | 70.58 | kJ/mol | Joback Method |
| log10ws | -4.16 | | Crippen Method |
| logp | 3.155 | | Crippen Method |
| mcvol | 236.840 | ml/mol | McGowan Method |
| pc | 1615.47 | kPa | Joback Method |
| rinpol | 2049.00 | | NIST Webbook |
| rinpol | 2049.00 | | NIST Webbook |
| tb | 747.07 | K | Joback Method |
| tc | 934.44 | K | Joback Method |
| tf | 475.39 | K | Joback Method |
| vc | 0.919 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 683.23 | J/mol×K | 747.07 | Joback Method |
| cpg | 697.23 | J/mol×K | 778.30 | Joback Method |
| cpg | 710.39 | J/mol×K | 809.53 | Joback Method |
| cpg | 722.71 | J/mol×K | 840.75 | Joback Method |
| cpg | 734.23 | J/mol×K | 871.98 | Joback Method |
| cpg | 744.97 | J/mol×K | 903.21 | Joback Method |
| cpg | 754.93 | J/mol×K | 934.44 | Joback Method |

# Sources

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|---|---|
| **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=U321478&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |