# Sarcosine, N-(2-trifluoromethylbenzoyl)-, tetradecyl ester

**Inchi:** InChI=1S/C25H38F3NO3/c1-3-4-5-6-7-8-9-10-11-12-13-16-19-32-23(30)20-29(2)24(31)2

**InchiKey:** ILZAMXCFJAJNMX-UHFFFAOYSA-N

**Formula:** C25H38F3NO3

**SMILES:** CCCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1C(F)(F)F

**Mol. weight [g/mol]:** 457.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -571.25 | kJ/mol | Joback Method |
| hf | -1221.20 | kJ/mol | Joback Method |
| hfus | 63.39 | kJ/mol | Joback Method |
| hvap | 88.38 | kJ/mol | Joback Method |
| log10ws | -7.86 | | Crippen Method |
| logp | 7.022 | | Crippen Method |
| mcvol | 363.650 | ml/mol | McGowan Method |
| pc | 912.18 | kPa | Joback Method |
| rinpol | 3027.00 | | NIST Webbook |
| tb | 940.24 | K | Joback Method |
| tc | 1151.76 | K | Joback Method |
| tf | 569.20 | K | Joback Method |
| vc | 1.419 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1215.82 | J/mol×K | 940.24 | Joback Method |
| cpg | 1233.34 | J/mol×K | 975.49 | Joback Method |
| cpg | 1249.63 | J/mol×K | 1010.75 | Joback Method |
| cpg | 1264.79 | J/mol×K | 1046.00 | Joback Method |
| cpg | 1278.91 | J/mol×K | 1081.26 | Joback Method |
| cpg | 1292.09 | J/mol×K | 1116.51 | Joback Method |
| cpg | 1304.40 | J/mol×K | 1151.76 | Joback Method |

# Sources

| | |
|---|---|
| **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=U321331&Units=SI |

# 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 |

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