# Sarcosine, N-(3-methoxybenzoyl)-, hexyl ester

**Inchi:** InChI=1S/C17H25NO4/c1-4-5-6-7-11-22-16(19)13-18(2)17(20)14-9-8-10-15(12-14)21-3/
**InchiKey:** YRAUKJCNOAUWLY-UHFFFAOYSA-N
**Formula:** C17H25NO4
**SMILES:** CCCCCCOC(=O)CN(C)C(=O)c1cccc(OC)c1
**Mol. weight [g/mol]:** 307.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -162.02 | kJ/mol | Joback Method |
| hf | -591.22 | kJ/mol | Joback Method |
| hfus | 42.03 | kJ/mol | Joback Method |
| hvap | 76.73 | kJ/mol | Joback Method |
| log10ws | -3.53 | | Crippen Method |
| logp | 2.891 | | Crippen Method |
| mcvol | 251.490 | ml/mol | McGowan Method |
| pc | 1674.16 | kPa | Joback Method |
| rinpol | 2426.00 | | NIST Webbook |
| rinpol | 2426.00 | | NIST Webbook |
| tb | 785.04 | K | Joback Method |
| tc | 984.36 | K | Joback Method |
| tf | 497.08 | K | Joback Method |
| vc | 0.946 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 745.50 | J/mol×K | 785.04 | Joback Method |
| cpg | 760.98 | J/mol×K | 818.26 | Joback Method |
| cpg | 775.41 | J/mol×K | 851.48 | Joback Method |
| cpg | 788.84 | J/mol×K | 884.70 | Joback Method |
| cpg | 801.27 | J/mol×K | 917.92 | Joback Method |
| cpg | 812.73 | J/mol×K | 951.14 | Joback Method |
| cpg | 823.25 | J/mol×K | 984.36 | 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=U321495&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 |