# Sarcosine, N-(4-methoxybenzoyl)-, propyl ester

**Inchi:** InChI=1S/C14H19NO4/c1-4-9-19-13(16)10-15(2)14(17)11-5-7-12(18-3)8-6-11/h5-8H,4,9-

**InchiKey:** QISXWZDVNHNMQB-UHFFFAOYSA-N

**Formula:** C14H19NO4

**SMILES:** CCCOC(=O)CN(C)C(=O)c1ccc(OC)cc1

**Mol. weight [g/mol]:** 265.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -187.28 | kJ/mol | Joback Method |
| hf | -529.30 | kJ/mol | Joback Method |
| hfus | 34.26 | kJ/mol | Joback Method |
| hvap | 70.05 | kJ/mol | Joback Method |
| log10ws | -2.27 | | Crippen Method |
| logp | 1.720 | | Crippen Method |
| mcvol | 209.220 | ml/mol | McGowan Method |
| pc | 2151.31 | kPa | Joback Method |
| rinpol | 2167.00 | | NIST Webbook |
| tb | 716.40 | K | Joback Method |
| tc | 920.18 | K | Joback Method |
| tf | 463.27 | K | Joback Method |
| vc | 0.777 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 579.34 | J/mol×K | 716.40 | Joback Method |
| cpg | 593.90 | J/mol×K | 750.36 | Joback Method |
| cpg | 607.52 | J/mol×K | 784.33 | Joback Method |
| cpg | 620.22 | J/mol×K | 818.29 | Joback Method |
| cpg | 632.01 | J/mol×K | 852.25 | Joback Method |
| cpg | 642.91 | J/mol×K | 886.21 | Joback Method |
| cpg | 652.92 | J/mol×K | 920.18 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U321420&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |