

Sarcosine, N-(4-methylbenzoyl)-, octyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C19H29NO3/c1-4-5-6-7-8-9-14-23-18(21)15-20(3)19(22)17-12-10-16(2)11-13- |
| InchiKey: | ZLSXDNDJIUKPSA-UHFFFAOYSA-N |
| Formula: | C19H29NO3 |
| SMILES: | CCCCCCCCOC(=O)CN(C)C(=O)c1ccc(C)cc1 |
| Mol. weight [g/mol]: | 319.44 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -40.18 | kJ/mol | Joback Method |
| hf | -500.28 | kJ/mol | Joback Method |
| hfus | 46.02 | kJ/mol | Joback Method |
| hvap | 78.77 | kJ/mol | Joback Method |
| log10ws | -4.72 | | Crippen Method |
| logp | 3.971 | | Crippen Method |
| mcvol | 273.800 | ml/mol | McGowan Method |
| pc | 1457.90 | kPa | Joback Method |
| rinpol | 2504.00 | | NIST Webbook |
| tb | 808.38 | K | Joback Method |
| tc | 1006.82 | K | Joback Method |
| tf | 497.39 | K | Joback Method |
| vc | 1.040 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 831.73 | J/molxK | 808.38 | Joback Method |
| cpg | 848.10 | J/molxK | 841.45 | Joback Method |
| cpg | 863.41 | J/molxK | 874.53 | Joback Method |
| cpg | 877.70 | J/molxK | 907.60 | Joback Method |
| cpg | 891.01 | J/molxK | 940.67 | Joback Method |
| cpg | 903.38 | J/molxK | 973.74 | Joback Method |
| cpg | 914.85 | J/molxK | 1006.82 | 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=U321220&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |

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 |
| hvac: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mccvol: | 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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<https://www.chemeo.com/cid/24-946-5/Sarcosine-N-4-methylbenzoyl-octyl-ester.pdf>

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