

Sarcosine, N-(3-methylbut-2-enoyl)-, octadecyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C26H49NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-30-26(29)23 |
| InchiKey: | GGXUXWAUGWEDIZ-UHFFFAOYSA-N |
| Formula: | C26H49NO3 |
| SMILES: | CCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C=C(C)C |
| Mol. weight [g/mol]: | 423.67 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -12.35 | kJ/mol | Joback Method |
| hf | -762.39 | kJ/mol | Joback Method |
| hfus | 69.40 | kJ/mol | Joback Method |
| hvap | 91.45 | kJ/mol | Joback Method |
| log10ws | -7.77 | | Crippen Method |
| logp | 7.216 | | Crippen Method |
| mcvol | 391.890 | ml/mol | McGowan Method |
| pc | 793.49 | kPa | Joback Method |
| tb | 940.92 | K | Joback Method |
| tc | 1155.26 | K | Joback Method |
| tf | 518.30 | K | Joback Method |
| vc | 1.520 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1329.94 | J/molxK | 940.92 | Joback Method |
| cpg | 1351.23 | J/molxK | 976.64 | Joback Method |
| cpg | 1371.16 | J/molxK | 1012.37 | Joback Method |
| cpg | 1389.84 | J/molxK | 1048.09 | Joback Method |
| cpg | 1407.35 | J/molxK | 1083.82 | Joback Method |
| cpg | 1423.76 | J/molxK | 1119.54 | Joback Method |
| cpg | 1439.17 | J/molxK | 1155.26 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U321528&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 |

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 |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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