

Propanamide, N,N-bis(2-ethylhexyl)-3-phenyl-

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|-----------------------------|--|
| Inchi: | InChI=1S/C25H43NO/c1-5-9-14-22(7-3)20-26(21-23(8-4)15-10-6-2)25(27)19-18-24-16-1 |
| InchiKey: | FHIAPOALXTYFEJ-UHFFFAOYSA-N |
| Formula: | C25H43NO |
| SMILES: | CCCCC(CC)CN(CC(CC)CCCC)C(=O)CCc1ccccc1 |
| Mol. weight [g/mol]: | 373.62 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 249.01 | kJ/mol | Joback Method |
| hf | -378.41 | kJ/mol | Joback Method |
| hfus | 52.12 | kJ/mol | Joback Method |
| hvap | 81.53 | kJ/mol | Joback Method |
| log10ws | -7.25 | | Crippen Method |
| logp | 6.881 | | Crippen Method |
| mcvol | 350.900 | ml/mol | McGowan Method |
| pc | 970.49 | kPa | Joback Method |
| rinpol | 2534.00 | | NIST Webbook |
| rinpol | 2534.00 | | NIST Webbook |
| tb | 863.51 | K | Joback Method |
| tc | 1061.30 | K | Joback Method |
| tf | 450.33 | K | Joback Method |
| vc | 1.339 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1142.60 | J/molxK | 863.51 | Joback Method |
| cpg | 1162.80 | J/molxK | 896.47 | Joback Method |
| cpg | 1181.78 | J/molxK | 929.44 | Joback Method |
| cpg | 1199.63 | J/molxK | 962.40 | Joback Method |
| cpg | 1216.42 | J/molxK | 995.37 | Joback Method |
| cpg | 1232.22 | J/molxK | 1028.33 | Joback Method |
| cpg | 1247.11 | J/molxK | 1061.30 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.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=U308216&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 |
| hvp: | 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 |
| rinp: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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