

Benzamide, 3-(trifluoromethyl)-N-undecyl-

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|-----------------------------|---|
| Inchi: | InChI=1S/C19H28F3NO/c1-2-3-4-5-6-7-8-9-10-14-23-18(24)16-12-11-13-17(15-16)19(20) |
| InchiKey: | PAUQOVSBPRVCJ-UHFFFAOYSA-N |
| Formula: | C19H28F3NO |
| SMILES: | CCCCCCCCCNC(=O)c1cccc(C(F)(F)F)c1 |
| Mol. weight [g/mol]: | 343.43 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -409.24 | kJ/mol | Joback Method |
| hf | -866.62 | kJ/mol | Joback Method |
| hfus | 47.14 | kJ/mol | Joback Method |
| hvap | 70.26 | kJ/mol | Joback Method |
| log10ws | -7.11 | | Crippen Method |
| logp | 5.966 | | Crippen Method |
| mvol | 271.670 | ml/mol | McGowan Method |
| pc | 1307.06 | kPa | Joback Method |
| rinpol | 2307.00 | | NIST Webbook |
| rinpol | 2307.00 | | NIST Webbook |
| tb | 764.40 | K | Joback Method |
| tc | 950.04 | K | Joback Method |
| tf | 449.61 | K | Joback Method |
| vc | 1.075 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 823.72 | J/mol×K | 764.40 | Joback Method |
| cpg | 840.03 | J/mol×K | 795.34 | Joback Method |
| cpg | 855.39 | J/mol×K | 826.28 | Joback Method |
| cpg | 869.86 | J/mol×K | 857.22 | Joback Method |
| cpg | 883.48 | J/mol×K | 888.16 | Joback Method |
| cpg | 896.33 | J/mol×K | 919.10 | Joback Method |
| cpg | 908.43 | J/mol×K | 950.04 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U407177&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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 |
| h vap: | 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 |
| r in pol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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