

Benzamide, N-decyl-N-methyl-2-trifluoromethyl-

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|----------------------|---|
| Inchi: | InChI=1S/C19H28F3NO/c1-3-4-5-6-7-8-9-12-15-23(2)18(24)16-13-10-11-14-17(16)19(20) |
| InchiKey: | ASZRFMWONOBQFH-UHFFFAOYSA-N |
| Formula: | C19H28F3NO |
| SMILES: | CCCCCCCCCN(C)C(=O)c1ccccc1C(F)(F)F |
| Mol. weight [g/mol]: | 343.43 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -387.85 | kJ/mol | Joback Method |
| hf | -852.56 | kJ/mol | Joback Method |
| hfus | 45.06 | kJ/mol | Joback Method |
| hvap | 65.87 | kJ/mol | Joback Method |
| log10ws | -6.49 | | Crippen Method |
| logp | 5.918 | | Crippen Method |
| mvol | 271.670 | ml/mol | McGowan Method |
| pc | 1293.00 | kPa | Joback Method |
| rinpol | 2151.00 | | NIST Webbook |
| rinpol | 2151.00 | | NIST Webbook |
| tb | 726.67 | K | Joback Method |
| tc | 907.83 | K | Joback Method |
| tf | 429.42 | K | Joback Method |
| vc | 1.058 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 804.19 | J/mol×K | 726.67 | Joback Method |
| cpg | 821.24 | J/mol×K | 756.86 | Joback Method |
| cpg | 837.31 | J/mol×K | 787.06 | Joback Method |
| cpg | 852.46 | J/mol×K | 817.25 | Joback Method |
| cpg | 866.75 | J/mol×K | 847.44 | Joback Method |
| cpg | 880.23 | J/mol×K | 877.64 | Joback Method |
| cpg | 892.96 | J/mol×K | 907.83 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U308534&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |

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 |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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