

Benzamide, N,N-diundecyl-2,3,4-trifluoro-

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| Inchi: | InChI=1S/C29H48F3NO/c1-3-5-7-9-11-13-15-17-19-23-33(24-20-18-16-14-12-10-8-6-4-2 |
| InchiKey: | YZMQZQDHBGAUPC-UHFFFAOYSA-N |
| Formula: | C29H48F3NO |
| SMILES: | CCCCCCCCCCCN(CCCCCCCCCC)C(=O)c1ccc(F)c(F)c1F |
| Mol. weight [g/mol]: | 483.69 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -325.75 | kJ/mol | Joback Method |
| hf | -1073.15 | kJ/mol | Joback Method |
| hfus | 77.60 | kJ/mol | Joback Method |
| hvap | 90.75 | kJ/mol | Joback Method |
| log10ws | -10.98 | | Crippen Method |
| logp | 9.608 | | Crippen Method |
| mvol | 412.570 | ml/mol | McGowan Method |
| pc | 696.18 | kPa | Joback Method |
| rinpol | 3153.00 | | NIST Webbook |
| rinpol | 3153.00 | | NIST Webbook |
| tb | 968.66 | K | Joback Method |
| tc | 1196.62 | K | Joback Method |
| tf | 564.74 | K | Joback Method |
| vc | 1.629 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1417.73 | J/mol×K | 968.66 | Joback Method |
| cpg | 1439.84 | J/mol×K | 1006.65 | Joback Method |
| cpg | 1460.41 | J/mol×K | 1044.65 | Joback Method |
| cpg | 1479.57 | J/mol×K | 1082.64 | Joback Method |
| cpg | 1497.40 | J/mol×K | 1120.63 | Joback Method |
| cpg | 1514.03 | J/mol×K | 1158.63 | Joback Method |
| cpg | 1529.56 | J/mol×K | 1196.62 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U308428&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |

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

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