

Benzamide, 3-fluoro-4-trifluoromethyl-N-(3-fluoro-4-trifluoromethylphenyl)

Inchi: InChI=1S/C26H27F8NO2/c1-2-3-4-5-6-7-8-9-14-35(23(36)17-10-12-19(21(27)15-17)25(26)11-13)/N
InchiKey: FPHCFODNQDLESL-UHFFFAOYSA-N
Formula: C26H27F8NO2
SMILES: CCCCCCCCCN(C(=O)c1ccc(C(F)(F)F)c(F)c1)C(=O)c1ccc(C(F)(F)F)c(F)c1
Mol. weight [g/mol]: 537.49

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -1345.52 | kJ/mol | Joback Method |
| hf | -1896.80 | kJ/mol | Joback Method |
| hfus | 65.65 | kJ/mol | Joback Method |
| hvap | 87.08 | kJ/mol | Joback Method |
| log10ws | -10.22 | | Crippen Method |
| logp | 8.426 | | Crippen Method |
| mvol | 356.960 | ml/mol | McGowan Method |
| pc | 912.73 | kPa | Joback Method |
| rinpol | 2448.00 | | NIST Webbook |
| rinpol | 2448.00 | | NIST Webbook |
| tb | 975.44 | K | Joback Method |
| tc | 1195.69 | K | Joback Method |
| tf | 627.59 | K | Joback Method |
| vc | 1.427 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1177.13 | J/molxK | 975.44 | Joback Method |
| cpg | 1191.79 | J/molxK | 1012.15 | Joback Method |
| cpg | 1205.53 | J/molxK | 1048.86 | Joback Method |
| cpg | 1218.46 | J/molxK | 1085.57 | Joback Method |
| cpg | 1230.74 | J/molxK | 1122.28 | Joback Method |
| cpg | 1242.50 | J/molxK | 1158.98 | Joback Method |
| cpg | 1253.86 | J/molxK | 1195.69 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U407913&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.cheméo.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 |
| 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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