

Benzamide, 2,6-difluoro-3-methyl-N-(2,6-difluoro-3-methylbenzyl)

Inchi: InChI=1S/C24H27F4NO2/c1-4-5-6-7-8-9-14-29(23(30)19-17(25)12-10-15(2)21(19)27)24
InchiKey: FSQGTRSCOAJXSS-UHFFFAOYSA-N
Formula: C24H27F4NO2
SMILES: CCCCCCN(C(=O)c1c(F)ccc(C)c1F)C(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 437.47

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -608.06 | kJ/mol | Joback Method |
| hf | -1076.52 | kJ/mol | Joback Method |
| hfus | 62.20 | kJ/mol | Joback Method |
| hvap | 89.81 | kJ/mol | Joback Method |
| log10ws | -8.79 | | Crippen Method |
| logp | 6.503 | | Crippen Method |
| mcvol | 321.700 | ml/mol | McGowan Method |
| pc | 1106.68 | kPa | Joback Method |
| rinpol | 2705.00 | | NIST Webbook |
| rinpol | 2705.00 | | NIST Webbook |
| tb | 949.02 | K | Joback Method |
| tc | 1162.65 | K | Joback Method |
| tf | 622.89 | K | Joback Method |
| vc | 1.266 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1026.47 | J/mol×K | 949.02 | Joback Method |
| cpg | 1040.75 | J/mol×K | 984.62 | Joback Method |
| cpg | 1053.91 | J/mol×K | 1020.23 | Joback Method |
| cpg | 1066.02 | J/mol×K | 1055.83 | Joback Method |
| cpg | 1077.14 | J/mol×K | 1091.44 | Joback Method |
| cpg | 1087.31 | J/mol×K | 1127.04 | Joback Method |
| cpg | 1096.61 | J/mol×K | 1162.65 | 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=U407761&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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