

2,4-Difluorobenzamide, N-pentyl-

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|-----------------------------|--|
| Inchi: | InChI=1S/C12H15F2NO/c1-2-3-4-7-15-12(16)10-6-5-9(13)8-11(10)14/h5-6,8H,2-4,7H2,1 |
| InchiKey: | CXDIYLXIWJAMDI-UHFFFAOYSA-N |
| Formula: | C12H15F2NO |
| SMILES: | CCCCCNC(=O)c1ccc(F)cc1F |
| Mol. weight [g/mol]: | 227.25 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -285.84 | kJ/mol | Joback Method |
| hf | -528.75 | kJ/mol | Joback Method |
| hfus | 32.96 | kJ/mol | Joback Method |
| hvap | 57.45 | kJ/mol | Joback Method |
| log10ws | -4.15 | | Crippen Method |
| logp | 2.885 | | Crippen Method |
| mcvol | 171.270 | ml/mol | McGowan Method |
| pc | 2304.74 | kPa | Joback Method |
| rinsol | 1668.00 | | NIST Webbook |
| tb | 613.18 | K | Joback Method |
| tc | 805.44 | K | Joback Method |
| tf | 380.23 | K | Joback Method |
| vc | 0.676 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 435.32 | J/mol×K | 613.18 | Joback Method |
| cpg | 448.75 | J/mol×K | 645.22 | Joback Method |
| cpg | 461.45 | J/mol×K | 677.27 | Joback Method |
| cpg | 473.45 | J/mol×K | 709.31 | Joback Method |
| cpg | 484.75 | J/mol×K | 741.35 | Joback Method |
| cpg | 495.40 | J/mol×K | 773.40 | Joback Method |
| cpg | 505.41 | J/mol×K | 805.44 | Joback Method |

Sources

| | |
|------------------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U358053&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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 |
| hvac: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mccol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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