# Benzamide, 3,4-difluoro-N-(3-methylbutyl)-

**Inchi:** InChI=1S/C12H15F2NO/c1-8(2)5-6-15-12(16)9-3-4-10(13)11(14)7-9/h3-4,7-8H,5-6H2,1-2
**InchiKey:** NPUJTGNHAWSHHG-UHFFFAOYSA-N
**Formula:** C12H15F2NO
**SMILES:** CC(C)CCNC(=O)c1ccc(F)c(F)c1
**Mol. weight [g/mol]:** 227.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -288.28 | kJ/mol | Joback Method |
| hf | -534.03 | kJ/mol | Joback Method |
| hfus | 29.43 | kJ/mol | Joback Method |
| hvap | 57.07 | kJ/mol | Joback Method |
| log10ws | -3.91 | | Crippen Method |
| logp | 2.741 | | Crippen Method |
| mcvol | 171.270 | ml/mol | McGowan Method |
| pc | 2322.54 | kPa | Joback Method |
| rinpol | 1693.00 | | NIST Webbook |
| rinpol | 1693.00 | | NIST Webbook |
| tb | 612.74 | K | Joback Method |
| tc | 808.57 | K | Joback Method |
| tf | 365.23 | K | Joback Method |
| vc | 0.670 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 435.76 | J/mol×K | 612.74 | Joback Method |
| cpg | 449.48 | J/mol×K | 645.38 | Joback Method |
| cpg | 462.45 | J/mol×K | 678.02 | Joback Method |
| cpg | 474.66 | J/mol×K | 710.66 | Joback Method |
| cpg | 486.16 | J/mol×K | 743.29 | Joback Method |
| cpg | 496.97 | J/mol×K | 775.93 | Joback Method |
| cpg | 507.10 | J/mol×K | 808.57 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U407791&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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

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