# Benzamide, 2,6-difluoro-3-methyl-N-isobutyl-

**Inchi:** InChI=1S/C12H15F2NO/c1-7(2)6-15-12(16)10-9(13)5-4-8(3)11(10)14/h4-5,7H,6H2,1-3H
**InchiKey:** JSSZGAHSICHRNG-UHFFFAOYSA-N
**Formula:** C12H15F2NO
**SMILES:** Cc1ccc(F)c(C(=O)NCC(C)C)c1F
**Mol. weight [g/mol]:** 227.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -297.91 | kJ/mol | Joback Method |
| hf | -545.50 | kJ/mol | Joback Method |
| hfus | 29.04 | kJ/mol | Joback Method |
| hvap | 57.73 | kJ/mol | Joback Method |
| log10ws | -3.97 | | Crippen Method |
| logp | 2.659 | | Crippen Method |
| mcvol | 171.270 | ml/mol | McGowan Method |
| pc | 2289.32 | kPa | Joback Method |
| rinpol | 1693.00 | | NIST Webbook |
| rinpol | 1693.00 | | NIST Webbook |
| tb | 617.72 | K | Joback Method |
| tc | 814.47 | K | Joback Method |
| tf | 377.75 | K | Joback Method |
| vc | 0.670 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 435.17 | J/mol×K | 617.72 | Joback Method |
| cpg | 448.69 | J/mol×K | 650.51 | Joback Method |
| cpg | 461.49 | J/mol×K | 683.30 | Joback Method |
| cpg | 473.57 | J/mol×K | 716.09 | Joback Method |
| cpg | 484.96 | J/mol×K | 748.88 | Joback Method |
| cpg | 495.67 | J/mol×K | 781.67 | Joback Method |
| cpg | 505.74 | J/mol×K | 814.47 | Joback Method |

# Sources

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|---|---|
| **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=U407736&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |