# Benzamide, 3,4-difluoro-N-butyl-

**Inchi:** InChI=1S/C11H13F2NO/c1-2-3-6-14-11(15)8-4-5-9(12)10(13)7-8/h4-5,7H,2-3,6H2,1H3,(
**InchiKey:** FFRNJJOBRPQELT-UHFFFAOYSA-N
**Formula:** C11H13F2NO
**SMILES:** CCCCNC(=O)c1ccc(F)c(F)c1
**Mol. weight [g/mol]:** 213.22

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -294.26 | kJ/mol | Joback Method |
| hf | -508.11 | kJ/mol | Joback Method |
| hfus | 30.37 | kJ/mol | Joback Method |
| hvap | 55.23 | kJ/mol | Joback Method |
| log10ws | -3.74 | | Crippen Method |
| logp | 2.495 | | Crippen Method |
| mcvol | 157.180 | ml/mol | McGowan Method |
| pc | 2532.82 | kPa | Joback Method |
| rinpol | 1633.00 | | NIST Webbook |
| tb | 590.30 | K | Joback Method |
| tc | 784.94 | K | Joback Method |
| tf | 368.96 | K | Joback Method |
| vc | 0.621 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 386.60 | J/mol×K | 590.30 | Joback Method |
| cpg | 399.37 | J/mol×K | 622.74 | Joback Method |
| cpg | 411.45 | J/mol×K | 655.18 | Joback Method |
| cpg | 422.84 | J/mol×K | 687.62 | Joback Method |
| cpg | 433.58 | J/mol×K | 720.06 | Joback Method |
| cpg | 443.69 | J/mol×K | 752.50 | Joback Method |
| cpg | 453.18 | J/mol×K | 784.94 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U407790&Units=SI |

# 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 |