

# Benzamide, 3,4-difluoro-N-(3,4-difluorobenzoyl)-N-butyl-

Inchi:	InChI=1S/C18H15F4NO2/c1-2-3-8-23(17(24)11-4-6-13(19)15(21)9-11)18(25)12-5-7-14(2
InchiKey:	FPFCKDFXNLDLIX-UHFFFAOYSA-N
Formula:	C18H15F4NO2
SMILES:	CCCCN(C(=O)c1ccc(F)c(F)c1)C(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]:	353.31

## Physical Properties

Property code	Value	Unit	Source
gf	-639.32	kJ/mol	Joback Method
hf	-929.74	kJ/mol	Joback Method
hfus	47.44	kJ/mol	Joback Method
hvap	75.13	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	4.326		Crippen Method
mcvol	237.160	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
tb	801.78	K	Joback Method
tc	1005.53	K	Joback Method
tf	530.23	K	Joback Method
vc	0.929	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.01	J/mol×K	801.78	Joback Method
cpg	694.56	J/mol×K	835.74	Joback Method
cpg	706.19	J/mol×K	869.70	Joback Method
cpg	716.94	J/mol×K	903.65	Joback Method
cpg	726.87	J/mol×K	937.61	Joback Method
cpg	736.01	J/mol×K	971.57	Joback Method
cpg	744.42	J/mol×K	1005.53	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U407808&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407808&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinp:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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