

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

Inchi:	InChI=1S/C15H9F4NO2/c1-20(14(21)8-2-4-10(16)12(18)6-8)15(22)9-3-5-11(17)13(19)7-
InchiKey:	OSYYQDSYZYVGTF-UHFFFAOYSA-N
Formula:	C15H9F4NO2
SMILES:	CN(C(=O)c1ccc(F)c(F)c1)C(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]:	311.23

## Physical Properties

Property code	Value	Unit	Source
gf	-664.58	kJ/mol	Joback Method
hf	-867.82	kJ/mol	Joback Method
hfus	39.67	kJ/mol	Joback Method
hvap	68.45	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.155		Crippen Method
mvol	194.890	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	1816.00		NIST Webbook
rinpol	1816.00		NIST Webbook
tb	733.14	K	Joback Method
tc	941.91	K	Joback Method
tf	496.42	K	Joback Method
vc	0.761	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.09	J/mol×K	733.14	Joback Method
cpg	532.49	J/mol×K	767.94	Joback Method
cpg	543.02	J/mol×K	802.73	Joback Method
cpg	552.73	J/mol×K	837.53	Joback Method
cpg	561.66	J/mol×K	872.32	Joback Method
cpg	569.83	J/mol×K	907.12	Joback Method
cpg	577.31	J/mol×K	941.91	Joback Method

# Sources

<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=U407805&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407805&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>hvap:</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>rinpola:</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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