

# Benzamide, 2,6-difluoro-3-methyl-N-(2,6-difluoro-3-methylbenzyl)

Inchi:	InChI=1S/C20H19F4NO2/c1-10(2)9-25(19(26)15-13(21)7-5-11(3)17(15)23)20(27)16-14(18)2
InchiKey:	BSSGBALEZFXGKP-UHFFFAOYSA-N
Formula:	C20H19F4NO2
SMILES:	<chem>Cc1ccc(F)c(C(=O)N(CC(C)C)C(=O)c2c(F)ccc(C)c2F)c1F</chem>
Mol. weight [g/mol]:	381.36

## Physical Properties

Property code	Value	Unit	Source
gf	-644.18	kJ/mol	Joback Method
hf	-999.24	kJ/mol	Joback Method
hfus	48.32	kJ/mol	Joback Method
hvap	80.52	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	4.798		Crippen Method
mvol	265.340	ml/mol	McGowan Method
pc	1463.49	kPa	Joback Method
rinpol	2262.00		NIST Webbook
rinpol	2262.00		NIST Webbook
tb	857.06	K	Joback Method
tc	1064.00	K	Joback Method
tf	562.81	K	Joback Method
vc	1.036	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.56	J/molxK	857.06	Joback Method
cpg	805.69	J/molxK	891.55	Joback Method
cpg	817.83	J/molxK	926.04	Joback Method
cpg	829.03	J/molxK	960.53	Joback Method
cpg	839.33	J/molxK	995.02	Joback Method
cpg	848.76	J/molxK	1029.51	Joback Method
cpg	857.38	J/molxK	1064.00	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=U407755&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407755&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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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