

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

<b>Inchi:</b>	InChI=1S/C23H37F2NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-26-23(27)20-16-17-21
<b>InchiKey:</b>	ITSGXZHXXWTGQN-UHFFFAOYSA-N
<b>Formula:</b>	C23H37F2NO
<b>SMILES:</b>	CCCCCCCCCCCCCCCCNC(=O)c1ccc(F)c(F)c1
<b>Mol. weight [g/mol]:</b>	381.54

## Physical Properties

Property code	Value	Unit	Source
gf	-193.22	kJ/mol	Joback Method
hf	-755.79	kJ/mol	Joback Method
hfus	61.45	kJ/mol	Joback Method
hvap	81.94	kJ/mol	Joback Method
log10ws	-8.76		Crippen Method
logp	7.176		Crippen Method
mvol	326.260	ml/mol	McGowan Method
pc	1014.89	kPa	Joback Method
rmpol	2865.00		NIST Webbook
rmpol	2865.00		NIST Webbook
tb	864.86	K	Joback Method
tc	1059.83	K	Joback Method
tf	504.20	K	Joback Method
vc	1.292	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1053.23	J/mol×K	864.86	Joback Method
cpg	1071.26	J/mol×K	897.35	Joback Method
cpg	1088.21	J/mol×K	929.85	Joback Method
cpg	1104.13	J/mol×K	962.34	Joback Method
cpg	1119.08	J/mol×K	994.84	Joback Method
cpg	1133.10	J/mol×K	1027.33	Joback Method
cpg	1146.24	J/mol×K	1059.83	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U407803&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407803&amp;Units=SI</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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