

# 2,5-Difluorobenzamide, N-(3-methylphenyl)-

<b>Inchi:</b>	InChI=1S/C14H11F2NO/c1-9-3-2-4-11(7-9)17-14(18)12-8-10(15)5-6-13(12)16/h2-8H,1H
<b>InchiKey:</b>	UWXXZDCUZZYARG-UHFFFAOYSA-N
<b>Formula:</b>	C14H11F2NO
<b>SMILES:</b>	Cc1cccc(NC(=O)c2cc(F)ccc2F)c1
<b>Mol. weight [g/mol]:</b>	247.24

## Physical Properties

Property code	Value	Unit	Source
gf	-166.22	kJ/mol	Joback Method
hf	-344.97	kJ/mol	Joback Method
hfus	31.79	kJ/mol	Joback Method
hvap	64.84	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.526		Crippen Method
mcvol	175.690	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1992.00		NIST Webbook
tb	690.60	K	Joback Method
tc	915.42	K	Joback Method
tf	441.71	K	Joback Method
vc	0.680	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.98	J/mol×K	690.60	Joback Method
cpg	467.03	J/mol×K	728.07	Joback Method
cpg	479.12	J/mol×K	765.54	Joback Method
cpg	490.27	J/mol×K	803.01	Joback Method
cpg	500.55	J/mol×K	840.48	Joback Method
cpg	509.98	J/mol×K	877.95	Joback Method
cpg	518.63	J/mol×K	915.42	Joback Method

# Sources

<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>
<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=U358045&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358045&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>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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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