

# 3,4-Difluorobenzamide, N-(2-iodo-4-methylphenyl)-

<b>Inchi:</b>	InChI=1S/C14H10F2INO/c1-8-2-5-13(12(17)6-8)18-14(19)9-3-4-10(15)11(16)7-9/h2-7H,1
<b>InchiKey:</b>	TUHXJUANSYYZKY-UHFFFAOYSA-N
<b>Formula:</b>	C14H10F2INO
<b>SMILES:</b>	Cc1ccc(NC(=O)c2ccc(F)c(F)c2)c(I)c1
<b>Mol. weight [g/mol]:</b>	373.14

## Physical Properties

Property code	Value	Unit	Source
gf	-117.73	kJ/mol	Joback Method
hf	-279.57	kJ/mol	Joback Method
hfus	35.81	kJ/mol	Joback Method
hvap	74.88	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.130		Crippen Method
mcvol	201.510	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	2534.00		NIST Webbook
tb	788.72	K	Joback Method
tc	1036.86	K	Joback Method
tf	512.29	K	Joback Method
vc	0.768	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.37	J/mol×K	788.72	Joback Method
cpg	505.44	J/mol×K	830.08	Joback Method
cpg	515.55	J/mol×K	871.43	Joback Method
cpg	524.77	J/mol×K	912.79	Joback Method
cpg	533.17	J/mol×K	954.14	Joback Method
cpg	540.82	J/mol×K	995.50	Joback Method
cpg	547.78	J/mol×K	1036.86	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=U358130&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358130&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>hvac:</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>mccol:</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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