

# 3-Chloro-2-fluorobenzamide, N-(4-fluorophenyl)-

**Inchi:** InChI=1S/C13H8ClF2NO/c14-11-3-1-2-10(12(11)16)13(18)17-9-6-4-8(15)5-7-9/h1-7H,(H

**InchiKey:** WYJLLCVXTJGFAB-UHFFFAOYSA-N

**Formula:** C13H8ClF2NO

**SMILES:** O=C(Nc1ccc(F)cc1)c1cccc(Cl)c1F

**Mol. weight [g/mol]:** 267.66

## Physical Properties

Property code	Value	Unit	Source
gf	-186.57	kJ/mol	Joback Method
hf	-340.07	kJ/mol	Joback Method
hfus	33.40	kJ/mol	Joback Method
hvap	67.00	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.870		Crippen Method
mcvol	173.840	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpol	2116.00		NIST Webbook
rinpol	2116.00		NIST Webbook
tb	705.15	K	Joback Method
tc	936.96	K	Joback Method
tf	460.36	K	Joback Method
vc	0.673	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.65	J/mol×K	705.15	Joback Method
cpg	438.02	J/mol×K	743.78	Joback Method
cpg	448.45	J/mol×K	782.42	Joback Method
cpg	458.01	J/mol×K	821.05	Joback Method
cpg	466.73	J/mol×K	859.69	Joback Method
cpg	474.67	J/mol×K	898.32	Joback Method
cpg	481.87	J/mol×K	936.96	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.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=U358133&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358133&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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