

# Benzamide, N-(4-fluorophenyl)-2-chloro-

<b>Inchi:</b>	InChI=1S/C13H9ClFNO/c14-12-4-2-1-3-11(12)13(17)16-10-7-5-9(15)6-8-10/h1-8H,(H,16)
<b>InchiKey:</b>	PMHCCURYPFIWPW-UHFFFAOYSA-N
<b>Formula:</b>	C13H9ClFNO
<b>SMILES:</b>	O=C(Nc1ccc(F)cc1)c1ccccc1Cl
<b>Mol. weight [g/mol]:</b>	249.67

## Physical Properties

Property code	Value	Unit	Source
gf	17.87	kJ/mol	Joback Method
hf	-132.49	kJ/mol	Joback Method
hfus	30.71	kJ/mol	Joback Method
hvap	67.16	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.731		Crippen Method
mcvol	172.070	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	2015.00		NIST Webbook
tb	700.90	K	Joback Method
tc	942.60	K	Joback Method
tf	447.25	K	Joback Method
vc	0.655	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.15	J/mol×K	700.90	Joback Method
cpg	432.28	J/mol×K	741.18	Joback Method
cpg	443.38	J/mol×K	781.47	Joback Method
cpg	453.49	J/mol×K	821.75	Joback Method
cpg	462.69	J/mol×K	862.03	Joback Method
cpg	471.04	J/mol×K	902.32	Joback Method
cpg	478.60	J/mol×K	942.60	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=U306978&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U306978&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>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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