

# 2-Chloro-4-fluorobenzamide

<b>Inchi:</b>	InChI=1S/C7H5ClFNO/c8-6-3-4(9)1-2-5(6)7(10)11/h1-3H,(H2,10,11)
<b>InchiKey:</b>	XIQZTMMWBKPFSE-UHFFFAOYSA-N
<b>Formula:</b>	C7H5ClFNO
<b>SMILES:</b>	NC(=O)c1ccc(F)cc1Cl
<b>Mol. weight [g/mol]:</b>	173.57
<b>CAS:</b>	88578-90-9

## Physical Properties

Property code	Value	Unit	Source
gf	-168.00	kJ/mol	Joback Method
hf	-264.86	kJ/mol	Joback Method
hfus	21.22	kJ/mol	Joback Method
hvap	55.73	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	1.578		Crippen Method
mcvol	111.290	ml/mol	McGowan Method
pc	4156.97	kPa	Joback Method
tb	559.30	K	Joback Method
tc	790.89	K	Joback Method
tf	383.81	K	Joback Method
vc	0.421	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.32	J/mol×K	559.30	Joback Method
cpg	237.92	J/mol×K	597.90	Joback Method
cpg	245.92	J/mol×K	636.50	Joback Method
cpg	253.35	J/mol×K	675.09	Joback Method
cpg	260.23	J/mol×K	713.69	Joback Method
cpg	266.58	J/mol×K	752.29	Joback Method
cpg	272.42	J/mol×K	790.89	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=C88578909&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C88578909&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>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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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