

# 3-Chloro-4-fluorobenzoic acid

<b>Other names:</b>	Benzoic acid, 3-chloro-4-fluoro-
<b>Inchi:</b>	InChI=1S/C7H4ClFO2/c8-5-3-4(7(10)11)1-2-6(5)9/h1-3H,(H,10,11)
<b>InchiKey:</b>	PKTSBFXIHLYGEY-UHFFFAOYSA-N
<b>Formula:</b>	C7H4ClFO2
<b>SMILES:</b>	O=C(O)c1ccc(F)c(Cl)c1
<b>Mol. weight [g/mol]:</b>	174.56
<b>CAS:</b>	403-16-7

## Physical Properties

Property code	Value	Unit	Source
gf	-371.27	kJ/mol	Joback Method
hf	-450.88	kJ/mol	Joback Method
hfus	20.11	kJ/mol	Joback Method
hvap	61.77	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.177		Crippen Method
mcvol	107.180	ml/mol	McGowan Method
pc	4351.13	kPa	Joback Method
tb	578.95	K	Joback Method
tc	784.83	K	Joback Method
tf	361.37	K	Joback Method
vc	0.411	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.54	J/mol×K	578.95	Joback Method
cpg	227.48	J/mol×K	613.26	Joback Method
cpg	233.97	J/mol×K	647.58	Joback Method
cpg	240.04	J/mol×K	681.89	Joback Method
cpg	245.70	J/mol×K	716.20	Joback Method
cpg	250.97	J/mol×K	750.52	Joback Method
cpg	255.86	J/mol×K	784.83	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C403167&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C403167&amp;Units=SI</a>
<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>

# 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>hvpap:</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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