

# 4-Chloro-3-nitrobenzenesulfonyl fluoride

<b>Inchi:</b>	InChI=1S/C6H3ClFNO4S/c7-5-2-1-4(14(8,12)13)3-6(5)9(10)11/h1-3H
<b>InchiKey:</b>	AMGFGPCYAMRLHF-UHFFFAOYSA-N
<b>Formula:</b>	C6H3ClFNO4S
<b>SMILES:</b>	O=[N+]([O-])c1cc(S(=O)(=O)F)ccc1Cl
<b>Mol. weight [g/mol]:</b>	239.61
<b>CAS:</b>	349-04-2

## Physical Properties

Property code	Value	Unit	Source
gf	-546.94	kJ/mol	Joback Method
hf	-629.54	kJ/mol	Joback Method
hfus	34.57	kJ/mol	Joback Method
hvap	71.34	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	1.906		Crippen Method
mcvol	131.160	ml/mol	McGowan Method
pc	5044.23	kPa	Joback Method
tb	609.64	K	Joback Method
tc	845.31	K	Joback Method
tf	421.52	K	Joback Method
vc	0.538	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.34	J/molxK	609.64	Joback Method
cpg	289.06	J/molxK	648.92	Joback Method
cpg	297.06	J/molxK	688.20	Joback Method
cpg	304.34	J/molxK	727.48	Joback Method
cpg	310.89	J/molxK	766.75	Joback Method
cpg	316.72	J/molxK	806.03	Joback Method
cpg	321.84	J/molxK	845.31	Joback Method

# Sources

<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>
<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=C349042&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C349042&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>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>mccvol:</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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