

# 4-Amino-3-bromo-5-chlorobenzotrifluoride

<b>Inchi:</b>	InChI=1S/C7H4BrClF3N/c8-4-1-3(7(10,11)12)2-5(9)6(4)13/h1-2H,13H2
<b>InchiKey:</b>	OVJCOPVKCCJSFE-UHFFFAOYSA-N
<b>Formula:</b>	C7H4BrClF3N
<b>SMILES:</b>	Nc1c(Cl)cc(C(F)(F)F)cc1Br
<b>Mol. weight [g/mol]:</b>	274.47
<b>CAS:</b>	109919-26-8

## Physical Properties

Property code	Value	Unit	Source
gf	-421.17	kJ/mol	Joback Method
hf	-538.39	kJ/mol	Joback Method
hfus	23.27	kJ/mol	Joback Method
hvap	53.15	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.704		Crippen Method
mcvol	130.760	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
tb	571.88	K	Joback Method
tc	801.07	K	Joback Method
tf	409.80	K	Joback Method
vc	0.502	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.80	J/molxK	571.88	Joback Method
cpg	276.86	J/molxK	610.08	Joback Method
cpg	284.22	J/molxK	648.28	Joback Method
cpg	290.93	J/molxK	686.48	Joback Method
cpg	297.06	J/molxK	724.67	Joback Method
cpg	302.65	J/molxK	762.87	Joback Method
cpg	307.77	J/molxK	801.07	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=C109919268&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C109919268&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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