

# 4-Amino-3-bromo-5-nitrobenzotrifluoride

<b>Inchi:</b>	InChI=1S/C7H4BrF3N2O2/c8-4-1-3(7(9,10)11)2-5(6(4)12)13(14)15/h1-2H,12H2
<b>InchiKey:</b>	ZUZMWPRSGJTLHW-UHFFFAOYSA-N
<b>Formula:</b>	C7H4BrF3N2O2
<b>SMILES:</b>	<chem>Nc1c(Br)cc(C(F)(F)F)cc1[N+](=O)[O-]</chem>
<b>Mol. weight [g/mol]:</b>	285.02
<b>CAS:</b>	113170-71-1

## Physical Properties

Property code	Value	Unit	Source
gf	-373.69	kJ/mol	Joback Method
hf	-533.41	kJ/mol	Joback Method
hfus	30.43	kJ/mol	Joback Method
hvap	65.36	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	2.958		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	686.29	K	Joback Method
tc	934.88	K	Joback Method
tf	523.49	K	Joback Method
vc	0.535	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.20	J/molxK	686.29	Joback Method
cpg	330.93	J/molxK	727.72	Joback Method
cpg	337.92	J/molxK	769.15	Joback Method
cpg	344.24	J/molxK	810.59	Joback Method
cpg	349.98	J/molxK	852.02	Joback Method
cpg	355.19	J/molxK	893.45	Joback Method
cpg	359.97	J/molxK	934.88	Joback Method

# Sources

<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=C113170711&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C113170711&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>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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