2-Amino-6-chlorobenzothiazole

Other names:	2-Benzothiazolamine, 6-chloro- Benzothiazole, 2-amino-6-chloro- 6-chlorobenzothiazol-2-ylamine
Inchi:	InChI=1S/C7H5ClN2S/c8-4-1-2-5-6(3-4)11-7(9)10-5/h1-3H,(H2,9,10)
InchiKey:	VMNXKIDUTPOHPO-UHFFFAOYSA-N
Formula:	C7H5ClN2S
SMILES:	Nc1nc2ccc(Cl)cc2s1
Mol. weight [g/mol]:	184.65
CAS:	95-24-9

Physical Properties

Property code	Value	Unit	Source
chs	-4090.50 ± 4.00	kJ/mol	NIST Webbook
hfs	-1.40 ± 3.90	kJ/mol	NIST Webbook
log10ws	-3.12		Crippen Method
logp	2.532		Crippen Method
mcvol	119.120	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95249&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume