

2-Amino-6-bromobenzothiazole

Other names:	Benzothiazole, 2-amino-6-bromo-
Inchi:	InChI=1S/C7H5BrN2S/c8-4-1-2-5-6(3-4)11-7(9)10-5/h1-3H,(H2,9,10)
InchiKey:	VZEBSJIOUMDNLY-UHFFFAOYSA-N
Formula:	C7H5BrN2S
SMILES:	<chem>Nc1nc2ccc(Br)cc2s1</chem>
Mol. weight [g/mol]:	229.10
CAS:	15864-32-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Crippen Method
logp	2.641		Crippen Method
mcvol	124.380	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15864321&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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