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: Nc1nc2ccc(Br)cc2s1
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/ci990307l
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