4-Amino-2,1,3-benzothiadiazole

Other names:	2,1,3-Benzothiadiazol-4-amine
	2,1,3-Benzothiadiazole, 4-amino-
	2,1,3-Benzothiadiazole, 7-amino-
	4-Aminopiazthiole
	7-Amino-2,1,3-benzothiadiazole
	2,1,3-benzothiadiazol-4-ylamine
Inchi:	InChI=1S/C6H5N3S/c7-4-2-1-3-5-6(4)9-10-8-5/h1-3H,7H2
InchiKey:	DRLGIZIAMHIQHL-UHFFFAOYSA-N
Formula:	C6H5N3S
SMILES:	Nc1cccc2nsnc12
Mol. weight [g/mol]:	151.19
CAS:	767-64-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	1.273		Crippen Method
mcvol	102.770	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C767646&Units=SI

Legend

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