

4-Aminobenzo-2,1,3-thiadiazole

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:	<chem>Nc1cccc2nsnc12</chem>
Mol. weight [g/mol]:	151.19

Physical Properties

Property code	Value	Unit	Source
ie	8.27	eV	Cheméo Relay (1.0)
logp	1.273		Crippen Method
mcvol	102.770	ml/mol	McGowan Method
tb	566.43	K	Cheméo Relay (1.0)
tf	402.11	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C767646&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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