

2-Cyanomethyl-1,3-benzothiazole

Other names:	Benzothiazol-2-ylacetonitrile
Inchi:	InChI=1S/C9H6N2S/c10-6-5-9-11-7-3-1-2-4-8(7)12-9/h1-4H,5H2
InchiKey:	ZMZSYUSDGRJZNT-UHFFFAOYSA-N
Formula:	C9H6N2S
SMILES:	N#CCc1nc2ccccc2s1
Mol. weight [g/mol]:	174.22
CAS:	56278-50-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.47		Crippen Method
logp	2.362		Crippen Method
mcvol	126.460	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56278503&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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