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/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