

1,2,3-Benzothiadiazole

Inchi:	InChI=1S/C6H4N2S/c1-2-4-6-5(3-1)7-8-9-6/h1-4H
InchiKey:	FNQJDLTXOVEEFB-UHFFFAOYSA-N
Formula:	C6H4N2S
SMILES:	c1ccc2snnc2c1
Mol. weight [g/mol]:	136.17
CAS:	273-77-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.691		Crippen Method
mcvol	92.790	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C273778&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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