

N-cyclohexyl-2-benzothiazole sulfonamide

Inchi:	InChI=1S/C13H16N2O2S2/c16-19(17,15-10-6-2-1-3-7-10)13-14-11-8-4-5-9-12(11)18-13
InchiKey:	STSDHUBQQWBRBH-UHFFFAOYSA-N
Formula:	C13H16N2O2S2
SMILES:	O=S(=O)(NC1CCCCC1)c1nc2ccccc2s1
Mol. weight [g/mol]:	296.41
CAS:	16170-33-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	2.907		Crippen Method
mcvol	208.650	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16170335&Units=SI

Legend

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

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