

(2-Benzothiazolyl)-guanidine

Other names:	Guanidine, 2-benzothiazolyl- Benzothiazole guanidine benzothiazol-2-ylguanidine
Inchi:	InChI=1S/C8H8N4S/c9-7(10)12-8-11-5-3-1-2-4-6(5)13-8/h1-4H,(H4,9,10,11,12)
InchiKey:	QMHWARSFUCGGBK-UHFFFAOYSA-N
Formula:	C8H8N4S
SMILES:	<chem>N=C(N)Nc1nc2ccccc2s1</chem>
Mol. weight [g/mol]:	192.24
CAS:	2582-07-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.15		Crippen Method
logp	1.602		Crippen Method
mcvol	136.630	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2582072&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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