Guanidine, 2-benzothiazolyl-

Other names:	Benzothiazole guanidine
	Guanidine, 2-benzothiazolyl-
	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:	QMHWARSFUCGBJK-UHFFFAOYSA-N
Formula:	C8H8N4S
SMILES:	N=C(N)Nc1nc2ccccc2s1
Mol. weight [g/mol]:	192.25

Physical Properties

Property code	Value	Unit	Source
ie	7.96	eV	Cheméo Relay (1.0)
log10ws	-3.10		Cheméo Relay (1.0)
logp	1.602		Crippen Method
mcvol	136.630	ml/mol	McGowan Method
tb	603.27	K	Cheméo Relay (1.0)
tf	503.68	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2582072&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point