

Benzothiazole, 5-chloro-2-methyl-

Other names:	5-Chloro-2-methylbenzothiazole USAF ek-p-4382
Inchi:	InChI=1S/C8H6CINS/c1-5-10-7-4-6(9)2-3-8(7)11-5/h2-4H,1H3
InchiKey:	XCALAYIRFYALSX-UHFFFAOYSA-N
Formula:	C8H6CINS
SMILES:	Cc1nc2cc(Cl)ccc2s1
Mol. weight [g/mol]:	183.66
CAS:	1006-99-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.96		Crippen Method
logp	3.258		Crippen Method
mcvol	123.230	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=C1006991&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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