

6-Chloro-2-methyl-7-methylsulfamyl-benzothiatrizine

Inchi:	InChI=1S/C8H9ClN4O4S2/c1-10-18(14,15)7-4-8-6(3-5(7)9)11-12-13(2)19(8,16)17/h3-4,1
InchiKey:	PZTXTWSLNFNUDLW-UHFFFAOYSA-N
Formula:	C8H9ClN4O4S2
SMILES:	CNS(=O)(=O)c1cc2c(cc1Cl)N=NN(C)S2(=O)=O
Mol. weight [g/mol]:	324.76
CAS:	1917-30-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.99		Crippen Method
logp	0.881		Crippen Method
mcvol	193.000	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=C1917302&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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