2H-1,2,4-Benzothiadiazine-7-sulfonamide, 6-chloro-3,4-dihydro-N,N,2,4-tetramethyl-, 1,1-dioxide

Other names: Hydrochlorothiazide tetra-methyl derivative
Hydrochlorothiazide, tetramethyl
Hydrochlorothiazide, tetramethyl deriv.
Hydrochlorothiazide Me

Inchi: InChI=1S/C11H16ClN3O4S2/c1-13(2)20(16,17)10-6-11-9(5-8(10)12)14(3)7-15(4)21(11,1

InchiKey: QPVCMENCMBSJLZ-UHFFFAOYSA-N

Formula: C11H16ClN3O4S2

SMILES: CN1CN(C)S(=O)(=O)c2cc(S(=O)(=O)N(C)C)c(Cl)cc21

Mol. weight [g/mol]: 353.85

CAS: 55670-20-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.38		Crippen Method
logp	0.618		Crippen Method
mcvol	229.590	ml/mol	McGowan Method
rinpol	2966.00		NIST Webbook
rinpol	2966.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C55670207&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices