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

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

Inchi: InChI=1S/C12H16F3N3O4S2/c1-16(2)23(19,20)10-6-11-9(5-8(10)12(13,14)15)17(3)7-18

InchiKey: KPSCHPPMJKWGIA-UHFFFAOYSA-N

Formula: C12H16F3N3O4S2

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

Mol. weight [g/mol]: 387.40

CAS: 55670-17-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.80		Crippen Method
logp	0.984		Crippen Method
mcvol	236.750	ml/mol	McGowan Method
rinpol	2653.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55670172&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices