Hydroflumethiazide tetra-methyl derivative

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

Physical Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55670172&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices