

Polythiazide

Other names:	2H-1,2,4-Benzothiadiazine-7-sulfonamide, 6-chloro-3,4-dihydro-2-methyl-3-[[[(2,2,2-trifluoroethyl)thio]methyl]-, 1,1-dioxide Drenasil Nephрил P 2525 Renese 6-Chloro-3,4-dihydro-2-methyl-3-(((2,2,2-trifluoroethyl)thio)methyl)-2H-1,2,4-benzothiadiazine-7-sulfonamide, 1,1-dioxide NSC 108161
Inchi:	6-Chloro-3,4-dihydro-2-methyl-3-[[[(2,2,2-trifluoroethyl)thio]methyl]-2H-1,2,4-benzothiadiazine-7-sulfonamide, 1,1-dioxide (polythiazide)
InchiKey:	CYLWJCABXYDINA-UHFFFAOYSA-N
Formula:	C11H13ClF3N3O4S3
SMILES:	CN1C(CSCC(F)(F)F)Nc2cc(Cl)c(S(N)(=O)=O)cc2S1(=O)=O
Mol. weight [g/mol]:	439.88
CAS:	346-18-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	1.655		Crippen Method
mcvol	251.250	ml/mol	McGowan Method
rinpol	2380.00		NIST Webbook
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rinpol	2380.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	42.67	kJ/mol	493.20	NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C346189&Units=SI>

Legend

hfust: Enthalpy of fusion at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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