Ethoxzolamide

Other names:	2-Benzothiazolesulfonamide, 6-ethoxy- 452-35-7 6-Ethoxy-2-benzothiazolesulfonamide 6-Ethoxybenzothiazole-2-sulfonamide 6-Ethoxyzolamide 6-ethoxybenzothiazole-2-sulphonamide Benzothiazole, 6-ethoxy-2-sulfonamide- Cardrase Diuretic C Ethamide Ethoxazolamide Ethoxyzolamide Etoxzolamide Glaucotensil NSC 10679 Redupresin U-4191
Inchi:	InChI=1S/C9H10N2O3S2/c1-2-14-6-3-4-7-8(5-6)15-9(11-7)16(10,12)13/h3-5H,2H2,1H3,(
InchiKey:	OUZWUKMCLIBBOG-UHFFFAOYSA-N
Formula:	C9H10N2O3S2
SMILES:	CCOc1ccc2nc(S(N)(=O)=O)sc2c1
Mol. weight [g/mol]:	258.32
CAS:	452-35-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Aqueous Solubility Prediction Method
log10ws	-3.81		Estimated Solubility Method
logp	1.342		Crippen Method
mcvol	169.020	ml/mol	McGowan Method
rinpol	2578.00		NIST Webbook
rinpol	2578.00		NIST Webbook
tf	464.00 ± 1.00	K	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C452357&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
tf:	Normal melting (fusion) point