

Sumatriptan

Other names:	3-[2-(Dimethylamino)ethyl]-N-methylindole-5-methanesulfonamide 1H-Indole-5-methanesulfonamide, 3-[2-(dimethylamino)ethyl]-N-methyl-
Inchi:	Sumatriptan Base (or) 3-[2-(Dimethylamino) ethyl]-N-Methyl-1H-Indole-5-Methane Sulfonamide InChI=1S/C14H21N3O2S/c1-15-20(18,19)10-11-4-5-14-13(8-11)12(9-16-14)6-7-17(2)3/h
InchiKey:	KQKPFRSPSRPDEB-UHFFFAOYSA-N
Formula:	C14H21N3O2S
SMILES:	CNS(=O)(=O)Cc1ccc2[nH]cc(CCN(C)C)c2c1
Mol. weight [g/mol]:	295.40
CAS:	103628-46-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.02		Crippen Method
logp	0.839		Crippen Method
mcvol	227.230	ml/mol	McGowan Method
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103628462&Units=SI
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

Legend

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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