

Zonisamide

Other names:	1,2-Benzisoxazole-3-methanesulfonamide AD-810 3-(Sulfamoylmethyl)-1,2-benzisoxazole Aleviatin CI-912 Exceglan Excegram PD-110843 1,2-Benzisoxazol-3-ylmethanesulfonamide Zonegran
Inchi:	InChI=1S/C8H8N2O3S/c9-14(11,12)5-7-6-3-1-2-4-8(6)13-10-7/h1-4H,5H2,(H2,9,11,12)
InchiKey:	UBQNRHZMVUUOMG-UHFFFAOYSA-N
Formula:	C8H8N2O3S
SMILES:	NS(=O)(=O)Cc1noc2ccccc12
Mol. weight [g/mol]:	212.23
CAS:	68291-97-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.91		Crippen Method
logp	0.616		Crippen Method
mcvol	138.580	ml/mol	McGowan Method
rinpole	2022.90		NIST Webbook
rinpole	2022.90		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68291974&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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