

Zolamine

Inchi: InChI=1S/C15H21N3OS/c1-17(2)9-10-18(15-16-8-11-20-15)12-13-4-6-14(19-3)7-5-13/h4
InchiKey: KYBJXENQEZJILU-UHFFFAOYSA-N
Formula: C15H21N3OS
SMILES: COc1ccc(CN(CCN(C)C)c2nccs2)cc1
Mol. weight [g/mol]: 291.41
CAS: 1155-03-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.96		Crippen Method
logp	2.720		Crippen Method
mcvol	231.150	ml/mol	McGowan Method
rmpol	2193.00		NIST Webbook
rmpol	2193.00		NIST Webbook
rmpol	2193.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1155039&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rmpol: Non-polar retention indices

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