

RTI 17

Inchi:	InChI=1S/C15H15N3S/c1-3-18-13-9-5-4-8-12(13)17(2)15(19)11-7-6-10-16-14(11)18/h4-
InchiKey:	ZSLBEMKAJDJVND-UHFFFAOYSA-N
Formula:	C15H15N3S
SMILES:	CCN1c2ccccc2N(C)C(=S)c2cccnc21
Mol. weight [g/mol]:	269.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.71		Estimated Solubility Method
logp	3.365		Crippen Method
mcvol	205.820	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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