

Promazine M (ring)

Inchi:	InChI=1S/C16H18N2S/c1-12(17-2)11-18-13-7-3-5-9-15(13)19-16-10-6-4-8-14(16)18/h3-
InchiKey:	IJOZCCILCJIHOA-UHFFFAOYSA-N
Formula:	C16H18N2S
SMILES:	CNC(C)CN1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]:	270.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.39		Crippen Method
logp	3.897		Crippen Method
mcvol	214.230	ml/mol	McGowan Method
rinpola	2080.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R212650&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
rinpola:	Non-polar retention indices

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