

Prothipendyl

Other names:	10H-Pyrido[3,2-b][1,4]benzothiazine-10-propanamine, N,N-dimethyl- 10H-Pyrido[3,2-b][1,4]benzothiazine, 10-[3-(dimethylamino)propyl]- Dominal Largophren LG 206 MH 05101 Phrenotropin Timoval Timovan Tolnate Tumovan D 206 N,N-Dimethyl-10H-pyrido[3,2-b][1,4]benzothiazine-10-propanamine 10-(3-Dimethylaminopropyl)-10H-pyrido(3,2-b)(1,4)benzothiazine
Inchi:	InChI=1S/C16H19N3S/c1-18(2)11-6-12-19-13-7-3-4-8-14(13)20-15-9-5-10-17-16(15)19/h
InchiKey:	JTTAUPUMOLRVRA-UHFFFAOYSA-N
Formula:	C16H19N3S
SMILES:	CN(C)CCCN1c2ccccc2Sc2cccnc21
Mol. weight [g/mol]:	285.41
CAS:	303-69-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	3.636		Crippen Method
mcvol	224.210	ml/mol	McGowan Method
rinpol	2343.00		NIST Webbook
rinpol	2339.00		NIST Webbook
rinpol	2339.00		NIST Webbook
rinpol	2343.00		NIST Webbook
rinpol	2348.00		NIST Webbook
rinpol	2348.00		NIST Webbook
rinpol	2339.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C303695&Units=SI

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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