Promazine

Other names:	10-[3-(Dimethylamino)Propyl]phenothiazine
	10H-Phenothiazine-10-propanamine, N,N-dimethyl-
	3276 R. P.
	A 145
	Ampazine
	Berophen
	Esparin
	Liranol
	N,N-Dimethyl-3-(10H-phenothiazin-10-yl)-1-propanamine
	N-Dimethylamino-1-methylethyl thiodiphenylamine
	N-[3-(Dimethylamino)propyl]phenothiazine
	NSC 31447
	Neo-Hibernex
	Phenothiazine, 10-(1-dimethylaminopropyl)-
	Phenothiazine, 10-[3-(dimethylamino)propyl]-
	Prazin
	Prazine
	Promazin
	Promazina
	Promwill
	Protactyl
	RP 3276
	Romtiazin
	Sinophenin
	Sparine
	Tomil
	Verophen
	Wy 1094
Inchi:	InChI=1S/C17H20N2S/c1-18(2)12-7-13-19-14-8-3-5-10-16(14)20-17-11-6-4-9-15(17)19/h
InchiKey:	ZGUGWUXLJSTTMA-UHFFFAOYSA-N
Formula:	C17H20N2S
SMILES:	CN(C)CCCN1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]:	284.42
CAS:	58-40-2

Physical Properties

Property code	Value	Unit	Source

ie	7.20 ± 0.06	eV	NIST Webbook
ie	7.23 ± 0.12	eV	NIST Webbook
ie	8.22 ± 0.07	eV	NIST Webbook
log10ws	-4.30		Aqueous Solubility Prediction Method
logp	4.241		Crippen Method
mcvol	228.320	ml/mol	McGowan Method
rinpol	2330.00		NIST Webbook
rinpol	2315.00		NIST Webbook
rinpol	2316.00		NIST Webbook
rinpol	2313.00		NIST Webbook
rinpol	2369.00		NIST Webbook
rinpol	2335.00		NIST Webbook
rinpol	2316.00		NIST Webbook
rinpol	2329.00		NIST Webbook
rinpol	2316.00		NIST Webbook
rinpol	2304.50		NIST Webbook
rinpol	2329.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2326.00		NIST Webbook
rinpol	2367.00		NIST Webbook
rinpol	2327.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58402&Units=SI

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices