Promethazine

Other names:

(+/-)-Promethazine
(2-Dimethylamino-2-methyl)ethyl-N-dibenzoparathiazine
10-(2-(Dimethylamino)-2-methylethyl)phenothiazine
10-[2-(Dimethylamino)propyl]phenothiazine
10H-Phenothiazine-10-ethanamine, N,N,«alpha»-trimethyl-
10H-Phenothiazine-10-ethanamine, N,N,Â«alphaÂ»-trimethyl-
3277 RP
A-91033
Aprobit
Atosil
Avomine
Dimapp
Dimethylamino-isopropyl-phenthiazin
Diphergan
Diprazine
Diprozin
Fargan
Fenazil
Fenetazina
Hiberna
Histargan
Iergigan
Isophenergan
Lercigan
Lilly 01516
Lilly 1516
N,N-dimethyl-1-phenothiazin-10-ylpropan-2-amine
N-(2'-Dimethylamino-2'-methyl)ethylphenothiazine
N-Dimethylamino-2-methylethyl thiodiphenylamine
NCI-C60673
Phargan
Phenargan
Phenergan base
Phenothiazine, 10-[2-(dimethylamino)propyl]-
Phensedyl
Pilpophen
Proazamine
Procit
Promazinamide
Prometasin

	Prometazin
	Prometazine
	Promethazin
	Promezathine
	Prorex
	Protazine
	Prothazin
	Provigan
	Pyrethiazine
	RP 3277
	SKF 1498
	Tanidil
	Thiergan
	Vallergine
	WY 509
Inchi:	InChI=1S/C17H20N2S/c1-13(18(2)3)12-19-14-8-4-6-10-16(14)20-17-11-7-5-9-15(17)19/h
InchiKey:	PWWVAXIEGOYWEE-UHFFFAOYSA-N
Formula:	C17H20N2S
SMILES:	CC(CN1c2ccccc2Sc2ccccc21)N(C)C
Mol. weight [g/mol]:	284.42
CAS:	60-87-7

Physical Properties

Property code	Value	Unit	Source
ie	7.25 ± 0.10	eV	NIST Webbook
log10ws	-4.13		Aqueous Solubility Prediction Method
logp	4.239		Crippen Method
mcvol	228.320	ml/mol	McGowan Method
rinpol	2254.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2276.00		NIST Webbook
rinpol	2280.00		NIST Webbook
rinpol	2260.00		NIST Webbook
rinpol	2256.00		NIST Webbook
rinpol	2254.00		NIST Webbook
rinpol	2234.00		NIST Webbook
rinpol	2280.00		NIST Webbook
rinpol	2259.00		NIST Webbook
rinpol	2272.00		NIST Webbook

rinpol	2260.00	NIST Webbook
rinpol	2259.00	NIST Webbook
rinpol	2256.00	NIST Webbook
rinpol	2259.00	NIST Webbook

Sources

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=C60877&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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