Diethazine

Other names:	10H-Phenothiazine-10-ethanamine, N,N-diethyl-
	Phenothiazine, 10-[2-(diethylamino)ethyl]-
	Casantin
	Dolisina
	Eazamine
	Fourneau 2987
	N-[2'-(Diethylamino)ethyl]dibenzo-p-thiazine
	10-(2-Diethylaminoethyl)phenothiazine
	Diethazin
	N-(2'-Diethylaminoethyl)dibenzoparathiazine
	Lodibon
	2987 R.P.
	Eazaminum
	Ethylemin
	Parkazin
	RP-2987
	10(Beta-diethylaminoethyl)-phenothiazine
	N-(Diethylaminoethyl)thiodiphenylamine
Inchi:	InChI=1S/C18H22N2S/c1-3-19(4-2)13-14-20-15-9-5-7-11-17(15)21-18-12-8-6-10-16(18)2
InchiKey:	LURMIKVZJSMXQE-UHFFFAOYSA-N
Formula:	C18H22N2S
SMILES:	CCN(CC)CCN1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]:	298.45
CAS:	60-91-3

Physical Properties

Property code	Value	Unit	Source
ie	7.85 ± 0.07	eV	NIST Webbook
log10ws	-4.50		Crippen Method
logp	4.631		Crippen Method
mcvol	242.410	ml/mol	McGowan Method
rinpol	2380.00		NIST Webbook
rinpol	2377.00		NIST Webbook
rinpol	2377.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60913&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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