

Pyrathiazine

Other names:	10H-Phenothiazine, 10-[2-(1-pyrrolidiny)ethyl]- Phenothiazine, 10-[2-(1-pyrrolidiny)ethyl]- N-(«beta»-Pyrrolidinoethyl)phenothiazine Parathiazine (pharmaceutical) Parathiazine (DCI) Pyrrolidine, 1-(2-phenothiazin-10-ylethyl)- Pyrrolidine, 1-[2-(10H-phenothiazin-10-yl)ethyl]- 10-[2-(1-Pyrrolidiny)ethyl]phenothiazine Parathiazine Pyrrolidino-aethyl-phenthiazin 10-(2-(1-Pyrrolidyl)ethyl)phenothiazine
Inchi:	InChI=1S/C18H20N2S/c1-3-9-17-15(7-1)20(14-13-19-11-5-6-12-19)16-8-2-4-10-18(16)2
InchiKey:	KJKJUXGEMYCCJN-UHFFFAOYSA-N
Formula:	C18H20N2S
SMILES:	<chem>c1ccc2c(c1)Sc1cccc1N2CCN1CCCC1</chem>
Mol. weight [g/mol]:	296.43
CAS:	84-08-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.40		Crippen Method
logp	4.385		Crippen Method
mcvol	231.550	ml/mol	McGowan Method
rinpola	2536.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84082&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
rinpol:	Non-polar retention indices

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