Periciazine

Other names: 10-(3-(4-Hydroxypiperidino)propyl)phenothiazine-2-carbonitrile
10H-Phenothiazine-2-carbonitrile, 10-[3-(4-hydroxy-1-piperidinyl)propyl]-
2-Cyano-10-(3-(4-hydroxy-1-piperidyl)propyl)phenothiazine
2-Cyano-10-(3-(4-hydroxypiperidino)propyl)phenothiazine
4-Piperidinol, 1-(3-(2-cyano-10-phenothiazinyl)propyl)-
6909 RP
Aolept
Bayer 1409
Cyano-3 ((hydroxy-4 piperidyl-1)-3 propyl)-10 phenothiazine
F.I. 6145
IC 6002
Nelactil
Nemactil
Neulactil
Neuleptil
Periciazinum
Pericyazine
Phenothiazine-2-carbonitrile, 10-[3-(4-hydroxypiperidino)propyl]-
Piperocyanomazine
Propericiazine
RP 8908
RP 8909
SKF 20,716
WH 7508

Inchi: InChI=1S/C21H23N3OS/c22-15-16-6-7-21-19(14-16)24(18-4-1-2-5-20(18)26-21)11-3-10-
InchiKey: LUALIOATIOESLM-UHFFFAOYSA-N
Formula: C21H23N3OS
SMILES: N#Cc1ccc2c(c1)N(CCCN1CCC(O)CC1)c1ccccc1S2
Mol. weight [g/mol]: 365.49
CAS: 2622-26-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Aqueous Solubility Prediction Method
logp	4.008		Crippen Method
mcvol	281.070	ml/mol	McGowan Method

rinpol	3225.00		NIST Webbook
rinpol	3227.00		NIST Webbook
rinpol	3230.00		NIST Webbook
rinpol	3207.00		NIST Webbook
rinpol	3249.00		NIST Webbook
rinpol	3225.00		NIST Webbook
rinpol	3249.00		NIST Webbook
rinpol	3207.00		NIST Webbook
rinpol	3227.00		NIST Webbook
rinpol	3230.00		NIST Webbook
tf	375.75	K	Aqueous Solubility Prediction Method

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=C2622266&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

tf: Normal melting (fusion) point