

Phenothiazine-10-propionitrile

Other names:	10-(2-Cyanoethyl)phenothiazine 10H-Phenothiazine-10-propanenitrile 10-Beta-cyanoethylphenothiazine
Inchi:	InChI=1S/C15H12N2S/c16-10-5-11-17-12-6-1-3-8-14(12)18-15-9-4-2-7-13(15)17/h1-4,6-
InchiKey:	YYDIIBWHOHWIOM-UHFFFAOYSA-N
Formula:	C15H12N2S
SMILES:	N#CCCN1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]:	252.33
CAS:	1698-80-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.54		Crippen Method
logp	4.203		Crippen Method
mcvol	191.540	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1698802&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/93-612-9/Phenothiazine-10-propionitrile.pdf>

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