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
ie	7.95	eV	Cheméo Relay (1.0)
log10ws	-5.26		Cheméo Relay (1.0)
logp	4.203		Crippen Method
mcvol	191.540	ml/mol	McGowan Method
tf	390.13	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1698802&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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