

Phenothiazine-3-propionic acid, 10-methyl-, hydrazide

Inchi:	InChI=1S/C16H17N3OS/c1-19-12-4-2-3-5-14(12)21-15-10-11(6-8-13(15)19)7-9-16(20)18
InchiKey:	GCJQDMPGPYAJGD-UHFFFAOYSA-N
Formula:	C16H17N3OS
SMILES:	CN1c2ccccc2Sc2cc(CCC(=O)NN)ccc21
Mol. weight [g/mol]:	299.39
CAS:	116633-00-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.45		Crippen Method
logp	2.842		Crippen Method
mcvol	225.780	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116633002&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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