

N-propynyl-phenothiazine

Inchi:	InChI=1S/C15H11NS/c1-2-11-16-12-7-3-5-9-14(12)17-15-10-6-4-8-13(15)16/h3-10H,1H3
InchiKey:	XPAKUJKFJVHHY-UHFFFAOYSA-N
Formula:	C15H11NS
SMILES:	CC#CN1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]:	237.32
CAS:	4282-90-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.96		Crippen Method
logp	4.270		Crippen Method
mcvol	181.560	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=C4282900&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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<https://www.chemeo.com/cid/75-213-2/N-propynyl-phenothiazine.pdf>

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