

fenethazine

Inchi:	InChI=1S/C16H18N2S/c1-17(2)11-12-18-13-7-3-5-9-15(13)19-16-10-6-4-8-14(16)18/h3-
InchiKey:	PFAXACNYGZVKMX-UHFFFAOYSA-N
Formula:	C16H18N2S
SMILES:	CN(C)CCN1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]:	270.39
CAS:	522-24-7

Physical Properties

Property code	Value	Unit	Source
ie	8.25 ± 0.07	eV	NIST Webbook
log10ws	-3.66		Crippen Method
logp	3.851		Crippen Method
mcvol	214.230	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C522247&Units=SI

Legend

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

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