

Phenothiazine-10-carbonyl chloride

Other names:	10H-Phenothiazine-10-carbonyl chloride
Inchi:	InChI=1S/C13H8CINOS/c14-13(16)15-9-5-1-3-7-11(9)17-12-8-4-2-6-10(12)15/h1-8H
InchiKey:	MJRIZSDRKPPHTK-UHFFFAOYSA-N
Formula:	C13H8CINOS
SMILES:	O=C(Cl)N1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]:	261.73
CAS:	18956-87-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Crippen Method
logp	4.648		Crippen Method
mcvol	175.790	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=C18956871&Units=SI

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/113-294-0/Phenothiazine-10-carbonyl-chloride.pdf>

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