

Phenothiazine-10-carbonylchloride

Other names:	10H-Phenothiazine-10-carbonyl chloride
Inchi:	InChI=1S/C13H8ClNOS/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:	C13H8ClNOS
SMILES:	O=C(Cl)N1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]:	261.73

Physical Properties

Property code	Value	Unit	Source
ie	7.85	eV	Cheméo Relay (1.0)
log10ws	-5.16		Cheméo Relay (1.0)
logp	4.648		Crippen Method
mcvol	175.790	ml/mol	McGowan Method
tb	658.81	K	Cheméo Relay (1.0)
tf	402.00	K	Cheméo Relay (1.0)

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18956871&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point

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