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