N-(n-propyl)-phenothiazine

Inchi: InChI=1S/C15H15NS/c1-2-11-16-12-7-3-5-9-14(12)17-15-10-6-4-8-13(15)16/h3-10H,2,11
InchiKey: LNXZDZDPYBPHAM-UHFFFAOYSA-N
Formula: C15H15NS
SMILES: CCCN1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]: 241.35
CAS: 15375-48-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	4.699		Crippen Method
mcvol	190.160	ml/mol	McGowan Method

Sources

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=C15375481&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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