Naphtho[1,2-b]thiophene, 8-methyl

Other names: Naphtho[1.2-b]thiophene, 8-methyl
Inchi: InChI=1S/C13H10S/c1-9-2-3-10-4-5-11-6-7-14-13(11)12(10)8-9/h2-8H,1H3
InchiKey: QCDXZSSPLMBBHB-UHFFFAOYSA-N
Formula: C13H10S
SMILES: Cc1ccc2ccc3ccsc3c2c1
Mol. weight [g/mol]: 198.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.31		Crippen Method
logp	4.363		Crippen Method
mcvol	152.000	ml/mol	McGowan Method
rinpol	312.90		NIST Webbook
rinpol	315.80		NIST Webbook
rinpol	312.90		NIST Webbook
rinpol	315.80		NIST Webbook
rinpol	315.61		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R21578&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices