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

Inchi: InChI=1S/C13H10S/c1-9-8-14-12-7-6-10-4-2-3-5-11(10)13(9)12/h2-8H,1H3
InchiKey: WXEUSOFSFSDRLZ-UHFFFAOYSA-N
Formula: C13H10S
SMILES: Cc1csc2ccc3ccccc3c12
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	323.58		NIST Webbook
rinpol	320.76		NIST Webbook
rinpol	320.76		NIST Webbook
rinpol	323.58		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R21582&Units=SI
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

Legend

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

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