Naphtho[1,2-b]thiophene, 5-methyl

Inchi: InChI=1S/C13H10S/c1-9-8-10-6-7-14-13(10)12-5-3-2-4-11(9)12/h2-8H,1H3
InchiKey: NJHJQIOJJXKMMN-UHFFFAOYSA-N
Formula: C13H10S
SMILES: Cc1cc2ccsc2c2ccccc12
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	316.24		NIST Webbook
rinpol	316.24		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R193034&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.