

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

Inchi: InChI=1S/C13H10S/c1-9-8-12-11-5-3-2-4-10(11)6-7-13(12)14-9/h2-8H,1H3
InchiKey: CLKHXEFJFULCEH-UHFFFAOYSA-N
Formula: C13H10S
SMILES: Cc1cc2c(ccc3ccccc32)s1
Mol. weight [g/mol]: 198.28
CAS: 16587-35-2

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	318.27		NIST Webbook
rinpol	311.77		NIST Webbook
rinpol	316.28		NIST Webbook
rinpol	316.28		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C16587352&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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