

Naphtho[1,2-b]thiophene, 6-methyl

Inchi: InChI=1S/C13H10S/c1-9-3-2-4-12-11(9)6-5-10-7-8-14-13(10)12/h2-8H,1H3
InchiKey: IPLAXWSPPPDWTF-UHFFFAOYSA-N
Formula: C13H10S
SMILES: Cc1cccc2c1ccc1ccsc12
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	319.60		NIST Webbook
rinpol	317.11		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R21564&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

Latest version available from:

<https://www.chemeo.com/cid/74-675-1/Naphtho-1-2-b-thiophene-6-methyl.pdf>

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