

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

Other names:	6-Methylnaphtho[2,1-b]thiophene Naphtho[2.1-b]thiophene, 6-methyl
Inchi:	InChI=1S/C13H10S/c1-9-3-2-4-11-10(9)5-6-13-12(11)7-8-14-13/h2-8H,1H3
InchiKey:	YRAKDQXVAIUULD-UHFFFAOYSA-N
Formula:	C13H10S
SMILES:	Cc1cccc2c1ccc1sccc12
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	323.53		NIST Webbook
rinpol	321.26		NIST Webbook

Sources

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=R21617&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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