

Naphtho[1,2-b]thiophene, 8-methyl

Other names:	Naphtho[1.2-b]thiophene, 8-methyl
Inchi:	InChI=1S/C13H10S/c1-9-2-3-10-4-5-11-6-7-14-13(11)12(10)8-9/h2-8H,1H3
InchiKey:	QCDXZSSPLMBBHB-UHFFFAOYSA-N
Formula:	C13H10S
SMILES:	<chem>Cc1ccc2ccc3ccsc3c2c1</chem>
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	312.90		NIST Webbook
rinpol	315.80		NIST Webbook
rinpol	312.90		NIST Webbook
rinpol	315.80		NIST Webbook
rinpol	315.61		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R21578&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

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<https://www.chemeo.com/cid/80-017-4/Naphtho-1-2-b-thiophene-8-methyl.pdf>

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