

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

Other names:	5-Methylnaphtho[2,1-b]thiophene
Inchi:	InChI=1S/C13H10S/c1-9-8-13-12(6-7-14-13)11-5-3-2-4-10(9)11/h2-8H,1H3
InchiKey:	POXQFGLAZGCSQP-UHFFFAOYSA-N
Formula:	C13H10S
SMILES:	<chem>Cc1cc2sccc2c2ccccc12</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	306.53		NIST Webbook
rinpol	320.34		NIST Webbook
rinpol	306.26		NIST Webbook
rinpol	320.34		NIST Webbook
rinpol	306.26		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=R21603&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/80-023-7/Naphtho-2-1-b-thiophene-5-methyl.pdf>

Generated by Cheméo on 2025-12-06 02:41:00.288423086 +0000 UTC m=+4737057.818463763.

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