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

Other names:	Naphtho[2.1-b]thiophene, 8-methyl
Inchi:	InChI=1S/C13H10S/c1-9-2-3-10-4-5-13-11(6-7-14-13)12(10)8-9/h2-8H,1H3
InchiKey:	XPYMKFHKEJLLNZ-UHFFFAOYSA-N
Formula:	C13H10S
SMILES:	Cc1ccc2ccc3sccc3c2c1
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	319.86		NIST Webbook
rinpol	317.18		NIST Webbook
rinpol	319.86		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=R21635&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/40-932-2/Naphtho-2-1-b-thiophene-8-methyl.pdf

Generated by Cheméo on 2024-10-12 07:11:30.495412592 +0000 UTC m=+3297953.132381843.

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