3-Methylbenzo[b]naphtho[2,1-d]thiophene

Other names:	3-methylbenzo[b]naphtho[2,1-d]thiopene
	Benzo[b]naphtho[2,1]thiophene, 3-methyl
	Benzo[b]naphtho[2,1-d]thiophene, 3-methyl
Inchi:	InChI=1S/C17H12S/c1-11-6-8-13-12(10-11)7-9-15-14-4-2-3-5-16(14)18-17(13)15/h2-10H
InchiKey:	JESYLDJZJBANHW-UHFFFAOYSA-N
Formula:	C17H12S
SMILES:	Cc1ccc2c(ccc3c4ccccc4sc23)c1
Mol. weight [g/mol]:	248.34
CAS:	4567-45-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	5.516		Crippen Method
mcvol	188.900	ml/mol	McGowan Method
rinpol	406.20		NIST Webbook
rinpol	407.55		NIST Webbook
rinpol	406.53		NIST Webbook
rinpol	406.53		NIST Webbook
rinpol	406.20		NIST Webbook
rinpol	407.60		NIST Webbook
rinpol	407.70		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=C4567457&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices