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

Other names:	Benzo[b]naphtho[2,1-d]thiophene, 5-methyl
	Benzo[b]naphtho[2,1]thiophene, 5-methyl
Inchi:	InChI=1S/C17H12S/c1-11-10-15-13-7-4-5-9-16(13)18-17(15)14-8-3-2-6-12(11)14/h2-10H
InchiKey:	LCIWJCAUAOQCDL-UHFFFAOYSA-N
Formula:	C17H12S
SMILES:	Cc1cc2c3ccccc3sc2c2ccccc12
Mol. weight [g/mol]:	248.34
CAS:	4567-49-1

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	409.35		NIST Webbook
rinpol	409.35		NIST Webbook
rinpol	408.94		NIST Webbook
rinpol	408.94		NIST Webbook
rinpol	410.58		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=C4567491&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

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