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

Other names:	Benzo[b]naphtho[1,2-d]thiophene, 11-methyl
	Benzo[b]naphtho[1,2]thiophene, 11-methyl
Inchi:	InChI=1S/C17H12S/c1-11-5-4-8-14-16(11)17-13-7-3-2-6-12(13)9-10-15(17)18-14/h2-10H
InchiKey:	ZDMWKUISVKVZNB-UHFFFAOYSA-N
Formula:	C17H12S
SMILES:	Cc1cccc2sc3ccc4ccccc4c3c12
Mol. weight [g/mol]:	248.34
CAS:	84258-84-4

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	403.10		NIST Webbook
rinpol	404.15		NIST Webbook
rinpol	402.67		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84258844&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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