Benzo[b]naphtho[2,3-d]thiophene, 7-methyl-

Other names:	7-Methylbenzo[b]naphtho[2,3-d]thiophene
	7-Methylbenzo[b]naptho[2,3-d]thiophene
	7-Methylnaphtho(2,3-b)benzothiophene
	9-Methyl-11-thiabenzo(b)fluorene
	7-Methylnaphtho[2,3-b][1]benzothiophene
	Benzo[b]naphtho[2,3]thiophene, 7-methyl
Inchi:	InChI=1S/C17H12S/c1-11-5-4-6-12-9-15-13-7-2-3-8-16(13)18-17(15)10-14(11)12/h2-10H
InchiKey:	CKOZCPVQNQOFGX-UHFFFAOYSA-N
Formula:	C17H12S
SMILES:	Cc1cccc2cc3c(cc12)sc1ccccc13
Mol. weight [g/mol]:	248.34
CAS:	24964-09-8

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	414.72		NIST Webbook
rinpol	417.07		NIST Webbook
rinpol	415.57		NIST Webbook
rinpol	415.57		NIST Webbook
rinpol	414.72		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=C24964098&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