Benzo[b]thiophene, 2,7-dimethyl-

Other names:	2,7-Dimethylbenzo[b]thiophene
	2,7-Dimethyl-1-benzothiophene
	2,7-Dimethyl-benzothiophene
	Benzothiophene, 2,7-dimethyl
Inchi:	InChI=1S/C10H10S/c1-7-4-3-5-9-6-8(2)11-10(7)9/h3-6H,1-2H3
InchiKey:	DNEXCQLUONZSTB-UHFFFAOYSA-N
Formula:	C10H10S
SMILES:	Cc1cc2cccc(C)c2s1
Mol. weight [g/mol]:	162.25
CAS:	16587-40-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	3.518		Crippen Method
mcvol	129.190	ml/mol	McGowan Method
rinpol	241.50		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=C16587409&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