6-ethyl,2,4-dimethyl-dibenzothiophene

Inchi: InChI=1S/C16H16S/c1-4-12-6-5-7-13-14-9-10(2)8-11(3)15(14)17-16(12)13/h5-9H,4H2,1-
InchiKey: NFJPQZILIUEDOB-UHFFFAOYSA-N
Formula: C16H16S
SMILES: CCc1cccc2c1sc1c(C)cc(C)cc12
Mol. weight [g/mol]: 240.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.59		Crippen Method
logp	5.234		Crippen Method
mcvol	194.270	ml/mol	McGowan Method
rinpol	356.14		NIST Webbook
rinpol	356.14		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R436267&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.