1-Phenyldibenzothiophene

Inchi: InChI=1S/C18H12S/c1-2-7-13(8-3-1)14-10-6-12-17-18(14)15-9-4-5-11-16(15)19-17/h1-1
InchiKey: VMXRUUFRMHNVDM-UHFFFAOYSA-N
Formula: C18H12S
SMILES: c1ccc(-c2cccc3sc4ccccc4c23)cc1
Mol. weight [g/mol]: 260.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.44		Crippen Method
logp	5.721		Crippen Method
mcvol	198.690	ml/mol	McGowan Method
rinpol	387.94		NIST Webbook
rinpol	387.94		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=U314396&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

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