4-Phenyldibenzothiophene

Inchi:	InChI=1S/C18H12S/c1-2-7-13(8-3-1)14-10-6-11-16-15-9-4-5-12-17(15)19-18(14)16/h1-1
InchiKey:	BMCNAHBDZUYGJG-UHFFFAOYSA-N
Formula:	C18H12S
SMILES:	c1ccc(-c2cccc3c2sc2ccccc23)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	405.68		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=U314397&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

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