

3-Phenyldibenzothiophene

Inchi: InChI=1S/C18H12S/c1-2-6-13(7-3-1)14-10-11-16-15-8-4-5-9-17(15)19-18(16)12-14/h1-11
InchiKey: SLQWXGMHQCRWHC-UHFFFAOYSA-N
Formula: C18H12S
SMILES: c1ccc(-c2ccc3c(c2)sc2ccccc23)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
rinpola	421.07		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=R556480&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
rinpola: Non-polar retention indices

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<https://www.chemeo.com/cid/14-138-3/3-Phenyldibenzothiophene.pdf>

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