

Thiophene, 2,4-diphenyl-

Other names:	2,4-Diphenylthiophene
Inchi:	InChI=1S/C16H12S/c1-3-7-13(8-4-1)15-11-16(17-12-15)14-9-5-2-6-10-14/h1-12H
InchiKey:	FKHVUWRLXRMJLF-UHFFFAOYSA-N
Formula:	C16H12S
SMILES:	<chem>c1ccc(-c2csc(-c3ccccc3)c2)cc1</chem>
Mol. weight [g/mol]:	236.33
CAS:	3328-86-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.43		Crippen Method
logp	5.082		Crippen Method
mcvol	185.670	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C3328867&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/73-993-9/Thiophene-2-4-diphenyl.pdf>

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