

Thiophene, tetraphenyl-

Other names:	Tetraphenylthiophene Thionessal 2,3,4,5-Tetraphenylthiophene
Inchi:	InChI=1S/C28H20S/c1-5-13-21(14-6-1)25-26(22-15-7-2-8-16-22)28(24-19-11-4-12-20-24)
InchiKey:	MQFBWJOMLIHUDY-UHFFFAOYSA-N
Formula:	C28H20S
SMILES:	<chem>c1ccc(-c2sc(-c3ccccc3)c(-c3ccccc3)c2-c2ccccc2)cc1</chem>
Mol. weight [g/mol]:	388.52
CAS:	1884-68-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.64		Crippen Method
logp	8.416		Crippen Method
mcvol	307.230	ml/mol	McGowan Method

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=C1884680&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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