

Thiophene, 2,5-bis(1,1-dimethylethyl)-

Other names:	Thiophene, 2,5-di-tert-butyl- 2,5-Di-tert-butylthiophene
Inchi:	InChI=1S/C12H20S/c1-11(2,3)9-7-8-10(13-9)12(4,5)6/h7-8H,1-6H3
InchiKey:	ISYGRXKYALZEIS-UHFFFAOYSA-N
Formula:	C12H20S
SMILES:	CC(C)(C)c1ccc(C(C)(C)C)s1
Mol. weight [g/mol]:	196.35
CAS:	1689-77-6

Physical Properties

Property code	Value	Unit	Source
ie	7.85	eV	NIST Webbook
log10ws	-3.86		Crippen Method
logp	4.343		Crippen Method
mcvol	176.830	ml/mol	McGowan Method

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=C1689776&Units=SI

Legend

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

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