

Thiophene, 2,4-bis(1,1-dimethylethyl)-

Other names:	Thiophene, 2,4-di-tert-butyl- 2,4-Di-tert-butylthiophene
Inchi:	InChI=1S/C12H20S/c1-11(2,3)9-7-10(13-8-9)12(4,5)6/h7-8H,1-6H3
InchiKey:	UAEOZSDBIPKLPV-UHFFFAOYSA-N
Formula:	C12H20S
SMILES:	CC(C)(C)c1csc(C(C)(C)C)c1
Mol. weight [g/mol]:	196.35
CAS:	33369-81-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.86		Crippen Method
logp	4.343		Crippen Method
mcvol	176.830	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33369812&Units=SI
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

Legend

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

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