

Thiophene, 2,5-bis(2-methylpropyl)-

Other names:	2,5-bis (2-methylpropyl)-thiophene
Inchi:	InChI=1S/C12H20S/c1-9(2)7-11-5-6-12(13-11)8-10(3)4/h5-6,9-10H,7-8H2,1-4H3
InchiKey:	DUKLFSDDEVHMJB-UHFFFAOYSA-N
Formula:	C12H20S
SMILES:	CC(C)Cc1ccc(CC(C)C)s1
Mol. weight [g/mol]:	196.35
CAS:	54845-33-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.03		Crippen Method
logp	4.145		Crippen Method
mcvol	176.830	ml/mol	McGowan Method
rinpol	1533.00		NIST Webbook

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=C54845339&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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