

Thiophene, 2-(3-methylbutyl)-5-propyl-

Other names:	2-Isopentyl-5-propylthiophene
Inchi:	InChI=1S/C12H20S/c1-4-5-11-8-9-12(13-11)7-6-10(2)3/h8-10H,4-7H2,1-3H3
InchiKey:	AEAISDGNZHADFV-UHFFFAOYSA-N
Formula:	C12H20S
SMILES:	CCCc1ccc(CCC(C)C)s1
Mol. weight [g/mol]:	196.35
CAS:	54845-34-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	4.289		Crippen Method
mcvol	176.830	ml/mol	McGowan Method
rinpol	1439.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54845340&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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