

Thiophene, 2-methyl-5-propyl-

Other names:	2-Methyl-5-propylthiophene
Inchi:	InChI=1S/C8H12S/c1-3-4-8-6-5-7(2)9-8/h5-6H,3-4H2,1-2H3
InchiKey:	ZWLVQEKJYWJRM-UHFFFAOYSA-N
Formula:	C8H12S
SMILES:	CCc1ccc(C)s1
Mol. weight [g/mol]:	140.25
CAS:	33933-73-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.93		Crippen Method
logp	3.009		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
rinpol	1033.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1035.00		NIST Webbook
ripol	1314.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33933732&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

ripol: Polar retention indices

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