

Thiophene, 2-ethyl-5-propyl-

Other names:	2-Ethyl-5-propylthiophene
Inchi:	InChI=1S/C9H14S/c1-3-5-9-7-6-8(4-2)10-9/h6-7H,3-5H2,1-2H3
InchiKey:	DXZDTEKFDJNGCS-UHFFFAOYSA-N
Formula:	C9H14S
SMILES:	CCCc1ccc(CC)s1
Mol. weight [g/mol]:	154.27
CAS:	54244-74-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	3.263		Crippen Method
mcvol	134.560	ml/mol	McGowan Method
rinpol	1120.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1120.00		NIST Webbook

Sources

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=C54244745&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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<https://www.chemeo.com/cid/18-778-9/Thiophene-2-ethyl-5-propyl.pdf>

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