Thiophene, 2-butyl-5-ethyl-

Other names:	2-Butyl-5-ethylthiophene
Inchi:	InChI=1S/C10H16S/c1-3-5-6-10-8-7-9(4-2)11-10/h7-8H,3-6H2,1-2H3
InchiKey:	ORAPMLHUSQJCQH-UHFFFAOYSA-N
Formula:	C10H16S
SMILES:	CCCCc1ccc(CC)s1
Mol. weight [g/mol]:	168.30
CAS:	54411-06-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Crippen Method
logp	3.653		Crippen Method
mcvol	148.650	ml/mol	McGowan Method
rinpol	1222.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1224.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54411062&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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