

5-tert-butyl-2-ethylthiofuran

Inchi:	InChI=1S/C10H16OS/c1-5-12-9-7-6-8(11-9)10(2,3)4/h6-7H,5H2,1-4H3
InchiKey:	WTLHQBIJQMKPW-UHFFFAOYSA-N
Formula:	C10H16OS
SMILES:	CCSc1ccc(C(C)(C)C)o1
Mol. weight [g/mol]:	184.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.68		Crippen Method
logp	3.689		Crippen Method
mcvol	154.520	ml/mol	McGowan Method
rinpola	1157.00		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R157503&Units=SI

Legend

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

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