

2,5-Dimethyl-3-ethylfuran

Inchi:	InChI=1S/C8H12O/c1-4-8-5-6(2)9-7(8)3/h5H,4H2,1-3H3
InchiKey:	XDCCUETYAWEEOS-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	CCc1cc(C)oc1C
Mol. weight [g/mol]:	124.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.96		Crippen Method
logp	2.459		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
rinpol	1054.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R643920&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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