5-methyl-2-propylfuran

Other names:	2-Methyl-5-propylfuran
	5-methyl-2-n-propylfuran
Inchi:	InChI=1S/C8H12O/c1-3-4-8-6-5-7(2)9-8/h5-6H,3-4H2,1-2H3
InchiKey:	XPYQVFYTBQVKIS-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	CCCc1ccc(C)o1
Mol. weight [g/mol]:	124.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.90		Crippen Method
logp	2.541		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
rinpol	891.00		NIST Webbook
ripol	1085.00		NIST Webbook
ripol	1064.00		NIST Webbook
ripol	1085.00		NIST Webbook
ripol	1102.00		NIST Webbook
ripol	1086.00		NIST Webbook
ripol	1086.00		NIST Webbook
ripol	1088.00		NIST Webbook
ripol	1086.00		NIST Webbook
ripol	1114.00		NIST Webbook
ripol	1102.00		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=R282694&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
ripol:	Polar retention indices