3(4)-methyl-2-n-propylfuran

Inchi:	InChI=1S/C8H12O/c1-3-4-8-7(2)5-6-9-8/h5-6H,3-4H2,1-2H3
InchiKey:	GJQIESIPKYWANO-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	CCCc1occc1C
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
ripol	1105.00		NIST Webbook
ripol	1105.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R296881&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices

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