

2-Butanoyl-5-methylfuran

Other names:	Furan, 2-butanoyl-5-methyl
Inchi:	InChI=1S/C9H12O2/c1-3-4-8(10)9-6-5-7(2)11-9/h5-6H,3-4H2,1-2H3
InchiKey:	IFHKZUYQKMDHIN-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	CCCC(=O)c1ccc(C)o1
Mol. weight [g/mol]:	152.19
CAS:	90673-55-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.18		Crippen Method
logp	2.571		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
rinpol	1192.00		NIST Webbook
rinpol	1192.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1748.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90673555&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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