

Furan, 2-acetyl-3-methyl

Other names:	2-acetyl-3-methylfuran
Inchi:	InChI=1S/C7H8O2/c1-5-3-4-9-7(5)6(2)8/h3-4H,1-2H3
InchiKey:	RJBGVAIXGHZIDY-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	CC(=O)c1occc1C
Mol. weight [g/mol]:	124.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.34		Crippen Method
logp	1.791		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
ripol	1601.00		NIST Webbook
ripol	1601.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R211464&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
ripol:	Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/92-798-5/Furan-2-acetyl-3-methyl.pdf>

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