

1-Pentanone, 1-(2-furanyl)-

Other names:	Furan, 2-pentanoyl
Inchi:	InChI=1S/C9H12O2/c1-2-3-5-8(10)9-6-4-7-11-9/h4,6-7H,2-3,5H2,1H3
InchiKey:	HTOZHTBIOGGHDJ-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	CCCCC(=O)c1ccco1
Mol. weight [g/mol]:	152.19
CAS:	3194-17-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	2.652		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
rinpol	1180.00		NIST Webbook
rinpol	1180.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1747.00		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=C3194170&Units=SI

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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<https://www.chemeo.com/cid/81-451-1/1-Pentanone-1-2-furanyl.pdf>

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