1-Octanone, 1-(2-furanyl)-

Other names:	2-Octanoylfuran
	1-(2-Furyl)-1-octanone
	Furan, 2-octanoyl
Inchi:	InChI=1S/C12H18O2/c1-2-3-4-5-6-8-11(13)12-9-7-10-14-12/h7,9-10H,2-6,8H2,1H3
InchiKey:	OQMUCISCOICEGC-UHFFFAOYSA-N
Formula:	C12H18O2
SMILES:	CCCCCCCC(=O)c1ccco1
Mol. weight [g/mol]:	194.27
CAS:	5456-77-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.38		Crippen Method
logp	3.823		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
rinpol	1487.00		NIST Webbook
ripol	2062.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5456779&Units=SI
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

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