1-Butanone, 1-(2-furanyl)-

Other names:	2-Butanoylfuran
	1-(2-Furanil)butanone
	1(2-Furyl)butanone
	1-(2-furanyl)-1-butanone
	1-furan-2-ylbutan-1-one
Inchi:	InChI=1S/C8H10O2/c1-2-4-7(9)8-5-3-6-10-8/h3,5-6H,2,4H2,1H3
InchiKey:	GONWJZJNVDRECJ-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	CCCC(=O)c1ccco1
Mol. weight [g/mol]:	138.16
CAS:	4208-57-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.70		Crippen Method
logp	2.262		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
rinpol	1078.00		NIST Webbook
rinpol	1078.00		NIST Webbook
ripol	1640.00		NIST Webbook
ripol	1644.00		NIST Webbook
ripol	1640.00		NIST Webbook
ripol	1641.00		NIST Webbook
ripol	1641.00		NIST Webbook
ripol	1642.00		NIST Webbook
ripol	1644.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4208575&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