

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

Other names:	2-Butanone, 1-(2-furyl)- 1-(2'-Furyl)-2-butanone 1-(2-furanyl)-2-butanone 1-(2-Furfuryl)-1-propanone
Inchi:	InChI=1S/C8H10O2/c1-2-7(9)6-8-4-3-5-10-8/h3-5H,2,6H2,1H3
InchiKey:	GLDGYLKTISAERO-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	CCC(=O)Cc1ccco1
Mol. weight [g/mol]:	138.16
CAS:	4208-63-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.13		Crippen Method
logp	1.801		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
ripol	1575.00		NIST Webbook
ripol	1584.00		NIST Webbook
ripol	1585.00		NIST Webbook
ripol	1591.00		NIST Webbook
ripol	1575.00		NIST Webbook
ripol	1584.00		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=C4208633&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices

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