

1-(2-furyl)-2-propanone

Other names:	1-(2-furanyl)-2-propanone 2-furfuryl methyl ketone Furfuryl methyl ketone 1-(2-furyl)propan-2-one (Furyl-2)-1-propanone-2 2-furylacetone
Inchi:	InChI=1S/C7H8O2/c1-6(8)5-7-3-2-4-9-7/h2-4H,5H2,1H3
InchiKey:	IQOJTGSBENZIOL-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	CC(=O)Cc1ccco1
Mol. weight [g/mol]:	124.14
CAS:	6975-60-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.71		Crippen Method
logp	1.411		Crippen Method
mcpvol	97.470	ml/mol	McGowan Method
ripol	919.00		NIST Webbook
ripol	954.00		NIST Webbook
ripol	952.00		NIST Webbook
ripol	952.00		NIST Webbook
ripol	952.00		NIST Webbook
ripol	952.00		NIST Webbook
ripol	1546.00		NIST Webbook
ripol	1548.00		NIST Webbook
ripol	1546.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1502.00		NIST Webbook
ripol	1522.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1502.00		NIST Webbook
ripol	1512.00		NIST Webbook
ripol	1548.00		NIST Webbook
ripol	1525.00		NIST Webbook

ripol	1525.00	NIST Webbook
ripol	1525.00	NIST Webbook
ripol	1512.00	NIST Webbook
ripol	1513.00	NIST Webbook
ripol	1497.00	NIST Webbook
ripol	1488.00	NIST Webbook
ripol	1482.00	NIST Webbook
ripol	1524.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C6975606&Units=SI

Legend

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

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