

1-(2-furyl)-1,2-propanedione

Other names:	1,2-Propanedione, 1-(2-furanyl)- 1-(2-furanyl)-1,2-propadione 1-(2-furanyl)-1,2-propanedione 1-(2-furanyl)-1,2-propandione 1-(2-furyl)propane-1,2-dione
Inchi:	InChI=1S/C7H6O3/c1-5(8)7(9)6-3-2-4-10-6/h2-4H,1H3
InchiKey:	JXZJRYDTSDCGLO-UHFFFAOYSA-N
Formula:	C7H6O3
SMILES:	CC(=O)C(=O)c1ccco1
Mol. weight [g/mol]:	138.12
CAS:	1438-92-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.56		Crippen Method
logp	1.051		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
rinpol	1042.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1035.00		NIST Webbook
ripol	1746.00		NIST Webbook
ripol	1753.00		NIST Webbook
ripol	1772.00		NIST Webbook
ripol	1759.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1761.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1734.00		NIST Webbook
ripol	1753.00		NIST Webbook
ripol	1734.00		NIST Webbook
ripol	1746.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=C1438922&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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