1-(5-methyl-2-furanyl)-1,2-propandione

Other names:	1-(5-methyl-2-furyl)propane-1,2-dione
Inchi:	InChI=1S/C8H8O3/c1-6-2-3-8(11-6)4-7(10)5-9/h2-3,5H,4H2,1H3
InchiKey:	SNZHDDIHWUADMV-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	Cc1ccc(CC(=O)C=O)o1
Mol. weight [g/mol]:	152.15
CAS:	1197-20-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.46		Crippen Method
logp	0.899		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
ripol	1847.00		NIST Webbook
ripol	1847.00		NIST Webbook

Sources

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=C1197202&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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