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: 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=C1197202&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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