1-(5-methyl-2-furyl)-1,2-propanedione

Inchi: InChI=1S/C8H8O3/c1-5-3-4-7(11-5)8(10)6(2)9/h3-4H,1-2H3
InchiKey: CSILYJHAPLAXTQ-UHFFFAOYSA-N
Formula: C8H8O3
SMILES: CC(=O)C(=O)c1ccc(C)o1
Mol. weight [g/mol]: 152.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.04		Crippen Method
logp	1.360		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
rinpol	1155.00		NIST Webbook
ripol	1824.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1854.00		NIST Webbook
ripol	1857.00		NIST Webbook
ripol	1824.00		NIST Webbook
ripol	1853.00		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=R248010&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