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

Inchi: InChI=1S/C9H10O3/c1-3-7(10)9(11)8-5-4-6(2)12-8/h4-5H,3H2,1-2H3
InchiKey: CWBAEQPKINGRQH-UHFFFAOYSA-N
Formula: C9H10O3
SMILES: CCC(=O)C(=O)c1ccc(C)o1
Mol. weight [g/mol]: 166.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.46		Crippen Method
logp	1.750		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
ripol	1946.00		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=R491422&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