

# 2-(2-Methoxycarbonyl-ethyl)-4-methyl-5-pentyl-furan-3-carboxylic acid methyl ester

InChI: InChI=1S/C16H24O5/c1-5-6-7-8-12-11(2)21-13(9-10-14(17)19-3)15(12)16(18)20-4/h5-10

InChIKey: PVPQIQKYSSSTQU-UHFFFAOYSA-N

Formula: C16H24O5

SMILES: CCCCCc1c(C)oc(CCC(=O)OC)c1C(=O)OC

Mol. weight [g/mol]: 296.36

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.48		Crippen Method
logp	3.213		Crippen Method
mcvol	237.590	ml/mol	McGowan Method
rinpol	1938.00		NIST Webbook

## Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R247671&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

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