2-(2-Methoxycarbonyl-ethyl)-4-methyl-5-pentyl-fu
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/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=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