2-Furoic acid, 2-methylpentyl ester

Inchi: InChI=1S/C11H16O3/c1-3-5-9(2)8-14-11(12)10-6-4-7-13-10/h4,6-7,9H,3,5,8H2,1-2H3
InchiKey: UEKUSUXMYHSUFB-UHFFFAOYSA-N
Formula: C11H16O3
SMILES: CCCC(C)COC(=O)c1ccco1
Mol. weight [g/mol]: 196.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.30		Crippen Method
logp	2.873		Crippen Method
mcvol	159.700	ml/mol	McGowan Method
rinpol	1437.00		NIST Webbook

Sources

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=U355171&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices