2-Furoic acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C11H16O4/c1-9(5-7-13-2)8-15-11(12)10-4-3-6-14-10/h3-4,6,9H,5,7-8H2,1-2H3
InchiKey: JJEOLVABDZBQCJ-UHFFFAOYSA-N
Formula: C11H16O4
SMILES: COCCC(C)COC(=O)c1ccco1
Mol. weight [g/mol]: 212.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.39		Crippen Method
logp	2.109		Crippen Method
mcvol	165.570	ml/mol	McGowan Method
rinpol	1555.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U355173&Units=SI
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

Legend

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