2-Furoic acid, 3-methylbut-2-yl ester

Inchi: InChI=1S/C10H14O3/c1-7(2)8(3)13-10(11)9-5-4-6-12-9/h4-8H,1-3H3
InchiKey: FDAFQECLKXSQHQ-UHFFFAOYSA-N
Formula: C10H14O3
SMILES: CC(C)C(C)OC(=O)c1ccco1
Mol. weight [g/mol]: 182.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.99		Crippen Method
logp	2.481		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
rinpol	1262.00		NIST Webbook
rinpol	1262.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U355168&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.