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

Inchi: InChI=1S/C10H12O3/c1-8(2)5-7-13-10(11)9-4-3-6-12-9/h3-6H,7H2,1-2H3
InchiKey: VXJVHDAXAKXWMT-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: CC(C)=CCOC(=O)c1ccco1
Mol. weight [g/mol]: 180.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.98		Crippen Method
logp	2.403		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
rinpol	1342.00		NIST Webbook
rinpol	1342.00		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=U299233&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

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