2-Furoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C14H18O3/c1-4-5-7-12(10-11(2)3)17-14(15)13-8-6-9-16-13/h6,8-9,11-12H,4,1
InchiKey: PDHVXJXOYIMFBK-UHFFFAOYSA-N
Formula: C14H18O3
SMILES: CCC#CC(CC(C)C)OC(=O)c1ccco1
Mol. weight [g/mol]: 234.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.46		Crippen Method
logp	3.264		Crippen Method
mcvol	193.370	ml/mol	McGowan Method
rinpol	1586.00		NIST Webbook
rinpol	1586.00		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=U299237&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.