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:	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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299237&Units=SI

Legend

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

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