2-Furoic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C16H20O3/c1-5-7-13(4)14(10-9-12(2)3)19-16(17)15-8-6-11-18-15/h6,8,11,13-1

InchiKey: VFCORKFAUYEVFH-UHFFFAOYSA-N

Formula: C16H20O3

SMILES: C=C(C)C#CC(OC(=O)c1ccco1)C(C)CCC

Mol. weight [g/mol]: 260.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.15		Crippen Method
logp	3.821		Crippen Method
mcvol	217.250	ml/mol	McGowan Method
rinpol	1714.00		NIST Webbook
rinpol	1714.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299239&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.