2-Furoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C11H12O3/c1-3-6-9(4-2)14-11(12)10-7-5-8-13-10/h5,7-9H,4H2,1-2H3
InchiKey: LZUDSPTZAZICSK-UHFFFAOYSA-N
Formula: C11H12O3
SMILES: CC#CC(CC)OC(=O)c1ccco1
Mol. weight [g/mol]: 192.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.45		Crippen Method
logp	2.238		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
rinpol	1397.00		NIST Webbook
rinpol	1397.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299235&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.