2-Furoic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C9H8O3/c1-3-7(2)12-9(10)8-5-4-6-11-8/h1,4-7H,2H3
InchiKey: JYIATTCFRNWMAJ-UHFFFAOYSA-N
Formula: C9H8O3
SMILES: C#CC(C)OC(=O)c1ccco1
Mol. weight [g/mol]: 164.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.61		Crippen Method
logp	1.458		Crippen Method
mcvol	122.920	ml/mol	McGowan Method
rinpol	988.00		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=U299232&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