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:	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=U299232&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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