2-Furoic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C10H8O3/c1-2-3-4-7-13-10(11)9-6-5-8-12-9/h1,3-6,8H,7H2
InchiKey: FSBJYDJWNUJZJO-UHFFFAOYSA-N
Formula: C10H8O3
SMILES: C#CC=CCOC(=O)c1ccco1
Mol. weight [g/mol]: 176.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.77		Crippen Method
logp	1.626		Crippen Method
mcvol	132.710	ml/mol	McGowan Method
rinpol	1355.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299234&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