

3-Furoic acid, anhydride with acetic acid

Inchi:	InChI=1S/C7H6O4/c1-5(8)11-7(9)6-2-3-10-4-6/h2-4H,1H3
InchiKey:	GRTHWCLJYVCSRM-UHFFFAOYSA-N
Formula:	C7H6O4
SMILES:	CC(=O)OC(=O)c1ccoc1
Mol. weight [g/mol]:	154.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.64		Crippen Method
logp	0.983		Crippen Method
mcvol	104.910	ml/mol	McGowan Method
rinsol	1114.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374899&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinsol:	Non-polar retention indices

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