

3,4-Furandimethanol, diacetate

Other names:	3,4-Bis(acetoxymethyl)furan 3,4-furan-3,4-diyl dimethyl diacetate
Inchi:	InChI=1S/C10H12O5/c1-7(11)14-5-9-3-13-4-10(9)6-15-8(2)12/h3-4H,5-6H2,1-2H3
InchiKey:	BNXMUMXYSWMXEC-UHFFFAOYSA-N
Formula:	C10H12O5
SMILES:	CC(=O)OCc1cocc1COC(C)=O
Mol. weight [g/mol]:	212.20
CAS:	30614-73-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.36		Crippen Method
logp	1.406		Crippen Method
mcvol	153.050	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30614734&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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