2-acetoxyfuranodiene

Inchi: InChI=1S/C17H22O3/c1-11-6-5-7-12(2)10-16-15(9-8-11)13(3)17(20-16)19-14(4)18/h7-8H
InchiKey: DDIISBOPYNGSCV-OHJCXFAUSA-N
Formula: C17H22O3
SMILES: CC(=O)Oc1oc2c(c1C)CC=C(C)CCC=C(C)C2
Mol. weight [g/mol]: 274.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.71		Crippen Method
logp	4.285		Crippen Method
mcvol	224.780	ml/mol	McGowan Method
rinpol	1884.00		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=R303850&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