2-hydroxyfuranodiene

Inchi: InChI=1S/C15H20O2/c1-10-4-5-14-12(3)9-17-15(14)8-11(2)7-13(16)6-10/h4,7,9,13,16H,
InchiKey: KWALLIHRTCHEFS-FJTWHMNQSA-N
Formula: C15H20O2
SMILES: CC1=CC(O)CC(C)=CCc2c(C)coc2C1
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.78		Crippen Method
logp	3.330		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
rinpol	1725.00		NIST Webbook
rinpol	1725.00		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=R337229&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

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