3-(5'-hydroxymethyl-2'-furyl)-2-phenyl-2-propenal

Inchi: InChI=1S/C14H12O3/c15-9-12(11-4-2-1-3-5-11)8-13-6-7-14(10-16)17-13/h1-9,16H,10H2
InchiKey: AYPZCVFZHFIVCL-WQLSENKSSA-N
Formula: C14H12O3
SMILES: O=CC(=Cc1ccc(CO)o1)c1ccccc1
Mol. weight [g/mol]: 228.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.65		Crippen Method
logp	2.511		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
rinpol	1965.00		NIST Webbook
rinpol	1965.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R389829&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.