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

Inchi: InChI=1S/C14H12O2/c1-11-7-8-14(16-11)9-13(10-15)12-5-3-2-4-6-12/h2-10H,1H3/b13-9
InchiKey: CXRNEDWJBURHEO-LCYFTJDESA-N
Formula: C14H12O2
SMILES: Cc1ccc(C=C(C=O)c2ccccc2)o1
Mol. weight [g/mol]: 212.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.98		Crippen Method
logp	3.328		Crippen Method
mcvol	168.040	ml/mol	McGowan Method
rinpol	1693.00		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=R389834&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