2-Phenyl-3-(2-furyl)-propenal

Other names:	Benzeneacetaldehyde, «alpha»-(2-furanylmethylene)- 3-(2-Furyl)-2-phenylpropenal
Inchi:	InChI=1S/C13H10O2/c14-10-12(9-13-7-4-8-15-13)11-5-2-1-3-6-11/h1-10H/b12-9-
InchiKey:	JPESOGFYFXAURP-XFXZXTDPSA-N
Formula:	C13H10O2
SMILES:	O=CC(=Cc1ccco1)c1ccccc1
Mol. weight [g/mol]:	198.22
CAS:	57568-60-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.51		Crippen Method
logp	3.019		Crippen Method
mcvol	153.950	ml/mol	McGowan Method
rinpol	1582.00		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=C57568602&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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