

1-Ethanone, 2-hydroxy, 1-(2-furyl)-2-benzoyl

Inchi:	InChI=1S/C13H10O4/c14-11(9-5-2-1-3-6-9)13(16)12(15)10-7-4-8-17-10/h1-8,13,16H
InchiKey:	BZRGEOFCSAEYJL-UHFFFAOYSA-N
Formula:	C13H10O4
SMILES:	O=C(c1ccccc1)C(O)C(=O)c1ccco1
Mol. weight [g/mol]:	230.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.13		Crippen Method
logp	1.706		Crippen Method
mcvol	165.690	ml/mol	McGowan Method
rinpol	1636.00		NIST Webbook
rinpol	1636.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R121069&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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