Ethanone, 1-[6-hydroxy-2-(1-methylethenyl)-7-benzofuranyl]-

Inchi: InChI=1S/C13H12O3/c1-7(2)11-6-9-4-5-10(15)12(8(3)14)13(9)16-11/h4-6,15H,1H2,2-3H

InchiKey: RFNNKKXNDZWUCP-UHFFFAOYSA-N

Formula: C13H12O3

SMILES: C=C(C)c1cc2ccc(O)c(C(C)=O)c2o1

Mol. weight [g/mol]: 216.23

CAS: 55682-75-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.46		Crippen Method
logp	3.374		Crippen Method
mcvol	164.120	ml/mol	McGowan Method
rinpol	1858.90		NIST Webbook
rinpol	1858.90		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55682752&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices