

Ethanone, 1,1'-(6-hydroxy-2,5-benzofurandiyl)bis-

Other names:	Euparone
Inchi:	InChI=1S/C12H10O4/c1-6(13)9-3-8-4-11(7(2)14)16-12(8)5-10(9)15/h3-5,15H,1-2H3
InchiKey:	FOXRXAILTBHLQA-UHFFFAOYSA-N
Formula:	C12H10O4
SMILES:	CC(=O)c1cc2cc(C(C)=O)c(O)cc2o1
Mol. weight [g/mol]:	218.21
CAS:	53947-86-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.88		Crippen Method
logp	2.544		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
rinpol	1640.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C53947867&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

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