

Yangonin

Other names:	2H-Pyran-2-one, 4-methoxy-6-[2-(4-methoxyphenyl)ethenyl]-, (E)- 2H-Pyran-2-one, 4-methoxy-6-(p-methoxystyryl)- 5-Hydroxy-3-methoxy-7-(p-methoxyphenyl)-2,4,6-heptatrienoic acid «gamma»-lactone 4-Methoxy-6-(«beta»-(p-anisyl)vinyl)-«alpha»-pyrone 4-Methoxy-6-(p-methoxystyryl)-2H-pyran-2-one (E)-4-Methoxy-6-(4-methoxystyryl)-2H-pyran-2-one
Inchi:	InChI=1S/C15H14O4/c1-17-12-6-3-11(4-7-12)5-8-13-9-14(18-2)10-15(16)19-13/h3-10H,1
InchiKey:	XLHIYUYCSMZCCC-VMPITWQZSA-N
Formula:	C15H14O4
SMILES:	<chem>COc1ccc(C=Cc2cc(OC)cc(=O)o2)cc1</chem>
Mol. weight [g/mol]:	258.27
CAS:	500-62-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.47		Crippen Method
logp	2.827		Crippen Method
mcvol	193.870	ml/mol	McGowan Method
rinpol	2678.20		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C500629&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

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