

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
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:

COc1ccc(C=Cc2cc(OC)cc(=O)o2)cc1

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

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C500629&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.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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<https://www.chemeo.com/cid/84-878-5/Yangonin.pdf>

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