

(E)-4-Methoxy-6-styryl-2H-pyran-2-one

Inchi: InChI=1S/C14H12O3/c1-16-13-9-12(17-14(15)10-13)8-7-11-5-3-2-4-6-11/h2-10H,1H3/b8
InchiKey: DKKJNZYHGRUXBS-BQYQJAHWSA-N
Formula: C14H12O3
SMILES: COc1cc(C=Cc2ccccc2)oc(=O)c1
Mol. weight [g/mol]: 228.24
CAS: 15345-89-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.35		Crippen Method
logp	2.819		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
rinpol	2353.50		NIST Webbook
rinpol	2353.50		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C15345898&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

Latest version available from:

<https://www.chemeo.com/cid/92-769-7/E-4-Methoxy-6-styryl-2H-pyran-2-one.pdf>

Generated by Cheméo on 2024-04-26 19:33:42.767070541 +0000 UTC m=+16449271.687647852.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.