

9H-Xanthen-9-one, 1-hydroxy-

Other names:	Xanthen-9-one, 1-hydroxy- 1-Hydroxyxanthone 1-Hydroxy-9H-xanthen-9-one
Inchi:	InChI=1S/C13H8O3/c14-9-5-3-7-11-12(9)13(15)8-4-1-2-6-10(8)16-11/h1-7,14H
InchiKey:	BNLRKUSVMCIOGU-UHFFFAOYSA-N
Formula:	C13H8O3
SMILES:	O=c1c2ccccc2oc2ccc(O)c12
Mol. weight [g/mol]:	212.20
CAS:	719-41-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.78		Crippen Method
logp	2.652		Crippen Method
mcvol	148.960	ml/mol	McGowan Method
rinpol	2006.00		NIST Webbook
rinpol	2006.00		NIST Webbook

Sources

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=C719415&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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