Trioxsalen

Other names:	2',4,8-Trimethylpsoralen
	2,5,9-Trimethyl-7H-furo(3,2-g)(1)benzopyran-7-one
	2,5,9-trimethylpyrano[5,6-f][1]benzoxol-7-one
	4,5',8-Trimethylpsoralen
	4,5',8-Trimethylpsoralene
	4,5,8-Trimethylpsoralen
	5-Benzofuranacrylic acid, 6-hydroxy-«beta»,2,7-trimethyl-, «delta»-lactone
	5-Benzofuranacrylic acid, 6-hydroxy-Â«betaÂ»,2,7-trimethyl-, Â«deltaÂ»-lactone
	7H-Furo[3,2-g][1]benzopyran-7-one, 2,5,9-trimethyl-
	Elder 8011
	NSC-71047
	Trimethylpsoralen
	Trioxalen
	Trioxsalin
	Trioxysalen
	Trisoralen
	Trixsalen
Inchi:	InChI=1S/C14H12O3/c1-7-4-12(15)17-14-9(3)13-10(6-11(7)14)5-8(2)16-13/h4-6H,1-3H3
InchiKey:	FMHHVULEAZTJMA-UHFFFAOYSA-N
Formula:	C14H12O3
SMILES:	Cc1cc2cc3c(C)cc(=O)oc3c(C)c2o1
Mol. weight [g/mol]:	228.24
CAS:	3902-71-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.28		Aqueous Solubility Prediction Method
logp	3.464		Crippen Method
mcvol	167.350	ml/mol	McGowan Method
rinpol	2155.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2155.00		NIST Webbook
tf	508.00 ± 1.00	K	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3902714&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
tf:	Normal melting (fusion) point