

Isopsoralen

Other names:	2H-Furo[2,3-h]chromen-2-one Angelecin 2H-Furo[2,3-H]-1-benzopyran-2-one Angecin Furo[5',4':7,8]coumarin 2-Propenoic acid, 3-(4-hydroxy-5-benzofuranyl)-, «delta»-lactone Furo(2,3-h)coumarin Angelicin Furo(5',4',7,8)coumarin 4-Hydroxy-5-benzofuranacrylic acid «gamma»-lactone 3-(4-Hydroxy-5-benzofuranyl)-2-propenoic acid «gamma»-lactone Isopsoralin NSC 404563
Inchi:	InChI=1S/C11H6O3/c12-10-4-2-7-1-3-9-8(5-6-13-9)11(7)14-10/h1-6H
InchiKey:	XDROKJSWHURZGO-UHFFFAOYSA-N
Formula:	C11H6O3
SMILES:	O=c1ccc2ccc3occc3c2o1
Mol. weight [g/mol]:	186.16
CAS:	523-50-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.97		Crippen Method
logp	2.539		Crippen Method
mcvol	125.080	ml/mol	McGowan Method
rinpol	1774.00		NIST Webbook
rinpol	1835.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C523502&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

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