

Methoxsalen

Other names: 5-Benzofuranacrylic acid, 6-hydroxy-7-methoxy-, «delta»-lactone
5-Benzofuranacrylic acid, 6-hydroxy-7-methoxy-, Â«deltaÂ»-lactone
7H-Furo[3,2-g][1]benzopyran-7-one, 9-methoxy-
8-MOP
8-MP
8-Methoxy-2',3',6,7-furocoumarin
8-Methoxy-4',5',6,7-furocoumarin
8-Methoxy-6,7-furanocoumarin
8-Methoxy-[furano-3'.2':6.7-coumarin]
8-Methoxyfuranocoumarin
8-Methoxypsoralen
8-Methoxypsoralene
9-Methoxy-7H-furo(3,2-g)benzopyran-7-one
9-Methoxy-7H-furo[3,2-g][1]benzopyran-7-one
9-Methoxy-7H-furo[3,2-g]chromen-7-one
9-methoxyfuro[3,2-g]chromen-7-one
9-methoxypsoralen
Ammodin
Ammoidin
Deltapsoralen
Geroxalen
Meladinin
Meladinine
Meladoxen
Meloxine
Methoxa-Dome
Methoxaten
Methoxsalene
NCI-C55903
NSC 45923
New-Meladinin
Oxsoralen
Oxsoralen lotion
Oxsoralen-Ultra
Oxypsoralen
Proralone-mop
Psoralon-mop
Puvalen
Puvamet
Uvadex

Vitpso
 Xanthotoxin
 Xanthotoxine
 Zanthotoxin
Inchi: InChI=1S/C12H8O4/c1-14-12-10-8(4-5-15-10)6-7-2-3-9(13)16-11(7)12/h2-6H,1H3
InchiKey: QXKHYNVANLEOEG-UHFFFAOYSA-N
Formula: C12H8O4
SMILES: COc1c2occc2cc2ccc(=O)oc12
Mol. weight [g/mol]: 216.19
CAS: 298-81-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.66		Estimated Solubility Method
log10ws	-3.58		Aqueous Solubility Prediction Method
logp	2.548		Crippen Method
mcpvol	145.040	ml/mol	McGowan Method
rinpol	2022.00		NIST Webbook
rinpol	2034.00		NIST Webbook
rinpol	2038.60		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	2034.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	2022.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	2040.00		NIST Webbook
rinpol	2034.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1990.00		NIST Webbook

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C298817&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
rinpola:	Non-polar retention indices

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