# 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 |
| mcvol | 145.040 | ml/mol | McGowan Method |
| rinpol | 1980.00 | | NIST Webbook |
| rinpol | 2040.00 | | NIST Webbook |
| rinpol | 2034.00 | | NIST Webbook |
| rinpol | 2034.00 | | NIST Webbook |
| rinpol | 1990.00 | | NIST Webbook |
| rinpol | 1990.00 | | NIST Webbook |
| rinpol | 2022.00 | | NIST Webbook |
| rinpol | 1980.00 | | NIST Webbook |
| rinpol | 2022.00 | | NIST Webbook |
| rinpol | 1990.00 | | NIST Webbook |
| rinpol | 2034.00 | | NIST Webbook |
| rinpol | 2038.60 | | NIST Webbook |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C298817&Units=SI |
| **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 |
| **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

# 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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