7H-Furo[3,2-g][1]benzopyran-7-one, 4-methoxy-

Other names: 4-Methoxy-7H-furo(3,2-g)(1)benzopyran-7-one
4-Methoxy-7H-furo[3,2-g]chromen-7-one
4-methoxyfuro[3,2-g]chromen-7-one
5-MOP
5-Methoxy-6,7-furanocoumarin
5-Methoxypsoralen
6-Hydroxy-4-methoxy-5-benzofuranacrylic acid, «gamma»-lactone
6-Hydroxy-4-methoxy-5-benzofuranacrylic acid, Â«gammaÂ»-lactone
Bergaptan
Bergapten
Bergaptene
Geralen
Heraclin
Majudin
NSC 95437
Psoraderm

Inchi: InChI=1S/C12H8O4/c1-14-12-7-2-3-11(13)16-10(7)6-9-8(12)4-5-15-9/h2-6H,1H3

InchiKey: BGEBZHIAGXMEMV-UHFFFAOYSA-N

Formula: C12H8O4

SMILES: COc1c2ccoc2cc2oc(=O)ccc12

Mol. weight [g/mol]: 216.19

CAS: 484-20-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Aqueous Solubility Prediction Method
logp	2.548		Crippen Method
mcvol	145.040	ml/mol	McGowan Method
rinpol	2048.00		NIST Webbook
rinpol	2075.00		NIST Webbook
rinpol	2062.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2060.70		NIST Webbook
rinpol	2061.00		NIST Webbook
rinpol	2062.00		NIST Webbook
rinpol	2048.00		NIST Webbook

rinpol	2061.00	NIST Webbook
rinpol	2062.00	NIST Webbook

Sources

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=C484208&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices