7-Methoxy-4-methylcoumarin

Other names:	2H-1-Benzopyran-2-one, 7-methoxy-4-methyl- Coumarin, 7-methoxy-4-methyl- Herniarin, 4-methyl- 4-Methyl-7-methoxycoumarin 4-Methylherniarin 2(1H)-Benzopyran-2-one, 7-methoxy-4-methyl
Inchi:	InChI=1S/C11H10O3/c1-7-5-11(12)14-10-6-8(13-2)3-4-9(7)10/h3-6H,1-2H3
InchiKey:	UDFPKNSWSYBIHO-UHFFFAOYSA-N
Formula:	C11H10O3
SMILES:	COc1ccc2c(C)cc(=O)oc2c1
Mol. weight [g/mol]:	190.20
CAS:	2555-28-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.03		Crippen Method
logp	2.110		Crippen Method
mcvol	140.240	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2555284&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume