

7-Methoxyflavone

Other names:	4H-1-Benzopyran-4-one, 7-methoxy-2-phenyl-Flavone, 7-methoxy-7-Methoxyflavanone
Inchi:	InChI=1S/C16H12O3/c1-18-12-7-8-13-14(17)10-15(19-16(13)9-12)11-5-3-2-4-6-11/h2-10
InchiKey:	QKNDCRMJDZLFEG-UHFFFAOYSA-N
Formula:	C16H12O3
SMILES:	<chem>COc1ccc2c(=O)cc(-c3ccccc3)oc2c1</chem>
Mol. weight [g/mol]:	252.26
CAS:	22395-22-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.15		Crippen Method
logp	3.469		Crippen Method
mcvol	186.930	ml/mol	McGowan Method
rinpol	2602.40		NIST Webbook
rinpol	2602.40		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C22395228&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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