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: COc1ccc2c(=O)cc(-c3ccccc3)oc2c1
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: 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
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