5,7-Dihydroxy-3,6,8-trimethoxyflavone

Other names:	4H-1-Benzopyran-4-one, 5,7-dihydroxy-3,6,8-trimethoxy-2-phenyl- Araneol
Inchi:	InChI=1S/C18H16O7/c1-22-16-11(19)10-12(20)17(23-2)14(9-7-5-4-6-8-9)25-15(10)18(24
InchiKey:	IAAZHANNYDYGRX-UHFFFAOYSA-N
Formula:	C18H16O7
SMILES:	COc1c(O)c(OC)c2oc(-c3ccccc3)c(OC)c(=O)c2c1O
Mol. weight [g/mol]:	344.32
CAS:	71479-92-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.49		Crippen Method
logp	2.897		Crippen Method
mcvol	238.590	ml/mol	McGowan Method
rinpol	3289.30		NIST Webbook
rinpol	3289.30		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C71479920&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