Tangeretin

Other names:	tangeritin
	Flavone, 5,6,7,8,4'-pentamethoxy
	5,6,7,8-tetramethoxy-2-(4-methoxyphenyl)-4-benzopyrone
Inchi:	InChI=1S/C20H20O7/c1-22-12-8-6-11(7-9-12)14-10-13(21)15-16(23-2)18(24-3)20(26-5)1
InchiKey:	ULSUXBXHSYSGDT-UHFFFAOYSA-N
Formula:	C20H20O7
SMILES:	COc1ccc(-c2cc(=O)c3c(OC)c(OC)c(OC)c(OC)c3o2)cc1
Mol. weight [g/mol]:	372.37
CAS:	481-53-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.63		Crippen Method
logp	3.503		Crippen Method
mcvol	266.770	ml/mol	McGowan Method
rinpol	3162.90		NIST Webbook
rinpol	3184.00		NIST Webbook
rinpol	3198.00		NIST Webbook
rinpol	3198.00		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=C481538&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