4',5,7,8-Tetramethoxyflavone

Other names: 5,7,8-Trimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one
Inchi: InChI=1S/C19H18O6/c1-21-12-7-5-11(6-8-12)14-9-13(20)17-15(22-2)10-16(23-3)18(24-4
InchiKey: DDGJUTBQQURRGE-UHFFFAOYSA-N
Formula: C19H18O6
SMILES: COc1ccc(-c2cc(=O)c3c(OC)cc(OC)c(OC)c3o2)cc1
Mol. weight [g/mol]: 342.34
CAS: 6601-66-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.51		Crippen Method
logp	3.494		Crippen Method
mcvol	246.810	ml/mol	McGowan Method
rinpol	3219.20		NIST Webbook
rinpol	3219.20		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=C6601667&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

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