2',3'-Dimethoxyflavone, TMS

Inchi: InChI=1S/C17H14O4/c1-19-15-9-5-7-12(17(15)20-2)16-10-13(18)11-6-3-4-8-14(11)21-16
InchiKey: OHEGMEUWGGBBHR-UHFFFAOYSA-N
Formula: C17H14O4
SMILES: COc1cccc(-c2cc(=O)c3ccccc3o2)c1OC
Mol. weight [g/mol]: 282.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.27		Crippen Method
logp	3.477		Crippen Method
mcvol	206.890	ml/mol	McGowan Method
rinpol	2515.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R579547&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices