DIMETHYLCHRYSIN

Other names: Flavone, 5,7-dimethoxy-
Chrysin - dimethyl ether
Dimethylchrysin
5,7-Dimethoxyflavone, TMS
Inchi: InChI=1S/C17H14O4/c1-19-12-8-15(20-2)17-13(18)10-14(21-16(17)9-12)11-6-4-3-5-7-11
InchiKey: JRFZSUMZAUHNSL-UHFFFAOYSA-N
Formula: C17H14O4
SMILES: COc1cc(OC)c2c(=O)cc(-c3ccccc3)oc2c1
Mol. weight [g/mol]: 282.29

Physical Properties

Property code	Value	Unit	Source
logp	3.477		Crippen Method
mcvol	206.890	ml/mol	McGowan Method
rinpol	2588.00		NIST Webbook
rinpol	2588.00		NIST Webbook
tf	419.02	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21392574&Units=SI

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point