CIRSILINEOL (5,4'-DIHYDROXY-6,7,3'-TRIMETHOXYFLAVONE)

Other names: Cirsilineol
Inchi: InChI=1S/C18H16O7/c1-22-13-6-9(4-5-10(13)19)12-7-11(20)16-14(25-12)8-15(23-2)18(2
InchiKey: VKOSQMWSWLZQPA-UHFFFAOYSA-N
Formula: C18H16O7
SMILES: COc1cc(-c2cc(=O)c3c(O)c(OC)c(OC)cc3o2)ccc1O
Mol. weight [g/mol]: 344.32

Physical Properties

Property code	Value	Unit	Source
logp	2.897		Crippen Method
mcvol	238.590	ml/mol	McGowan Method
rinpol	3343.50		NIST Webbook
rinpol	3343.50		NIST Webbook
tf	490.11	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41365326&Units=SI
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):

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point