Eupatorin

Inchi: InChI=1S/C18H16O7/c1-22-12-5-4-9(6-10(12)19)13-7-11(20)16-14(25-13)8-15(23-2)18(2
InchiKey: KLAOKWJLUQKWIF-UHFFFAOYSA-N
Formula: C18H16O7
SMILES: COc1ccc(-c2cc(=O)c3c(O)c(OC)c(OC)cc3o2)cc1O
Mol. weight [g/mol]: 344.32
CAS: 855-96-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.49		Crippen Method
logp	2.897		Crippen Method
mcvol	238.590	ml/mol	McGowan Method
rinpol	3422.30		NIST Webbook
rinpol	3422.30		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C855969&Units=SI

Legend

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