Kaempferol

Inchi: InChI=1S/C15H10O6/c16-8-3-1-7(2-4-8)15-14(20)13(19)12-10(18)5-9(17)6-11(12)21-15/
InchiKey: IYRMWMYZSQPJKC-UHFFFAOYSA-N
Formula: C15H10O6
SMILES: O=c1c(O)c(-c2ccc(O)cc2)oc2cc(O)cc(O)c12
Mol. weight [g/mol]: 286.24
CAS: 520-18-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Cheméo Relay (1.0)
logp	2.282		Crippen Method
mcvol	190.450	ml/mol	McGowan Method
tf	550.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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
tf: Normal melting (fusion) point

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