5,7-dihydroxy-3-(4-hydroxyphenyl)-4H-chromen-4

Other names: genistein
Inchi: InChI=1S/C15H10O5/c16-9-3-1-8(2-4-9)11-7-20-13-6-10(17)5-12(18)14(13)15(11)19/h1-
InchiKey: TZBJGXHYKVUXJN-UHFFFAOYSA-N
Formula: C15H10O5
SMILES: O=c1c(-c2ccc(O)cc2)coc2cc(O)cc(O)c12
Mol. weight [g/mol]: 270.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Cheméo Relay (1.0)
logp	2.577		Crippen Method
mcvol	184.580	ml/mol	McGowan Method
tf	575.05	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):
Solubility of Genistein in Water, Methanol, Ethanol, Propan-2-ol, 1-Butanol, and Ethyl Acetate from (280 to 330) K: https://www.doi.org/10.1021/je100261w
Dissociation Constants and Solubilities of Daidzein and Genistein in Different Solvents: https://www.doi.org/10.1021/je4010905

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point