

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, Diethyl Ether, and Ethyl Acetate from 12 to 25 °C:	https://www.doi.org/10.1021/je100261w
Dissociation Constants and Solubilities of Genistein 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

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