naringin

Other names:	(S)-7-(((2S,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-(((2S,3R,4R,5R,6S)-3,4,5-tr naringoside
Inchi:	InChI=1S/C27H32O14/c1-10-20(32)22(34)24(36)26(37-10)41-25-23(35)21(33)18(9-28)40
InchiKey:	DFPMSGMNTNDNHN-ZPHOTFPESA-N
Formula:	C27H32O14
SMILES:	CC1OC(OC2C(Oc3cc(O)c4c(c3)OC(c3ccc(O)cc3)CC4=O)OC(CO)C(O)C2O)C(O)C(O)C
Mol. weight [g/mol]:	580.54

Physical Properties

Property code	Value	Unit	Source
hfus	103.18	kJ/mol	Joback Method
logp	-1.165		Crippen Method
mcvol	389.070	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.96	J/mol×K	1801.06	Joback Method
cpg	1499.38	J/mol×K	1965.80	Joback Method
cpg	1479.15	J/mol×K	2130.54	Joback Method
cpg	1466.96	J/mol×K	2295.28	Joback Method
cpg	1469.56	J/mol×K	2460.02	Joback Method
cpg	1493.65	J/mol×K	2624.75	Joback Method
cpg	1545.96	J/mol×K	2789.49	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Solubilities of Naringin and Naringenin in Different Solvents and Dissociation Constants of Naringenin:	https://www.doi.org/10.1021/je501004g

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume