Flavone-3-rutinoside, 3,3',4',5,7-pentahydroxy

Other names:	rutoside
Inchi:	3-[[6-O-(6-deoxy-«alpha»-L-mannopyranosyl)-«beta»-D-glucopyranosyl]-oxy]-2-(3,4-dihy(rutin) InChI=1S/C27H30O16/c1-8-17(32)20(35)22(37)26(40-8)39-7-15-18(33)21(36)23(38)27(4
InchiKey:	IKGXIBQEEMLURG-UHFFFAOYSA-N
Formula:	C27H30O16
SMILES:	CC1OC(OCC2OC(Oc3c(-c4ccc(O)c(O)c4)oc4cc(O)cc(O)c4c3=O)C(O)C(O)C2O)C(O)C(O
Mol. weight [g/mol]:	610.52
CAS:	153-18-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.69		Crippen Method
logp	-1.687		Crippen Method
mcvol	396.510	ml/mol	McGowan Method

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=C153184&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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