Esculetin

Other names:	2H-1-Benzopyran-2-one, 6,7-dihydroxy-
	6,7-dihydroxy-2-benzopyrone
	6,7-dihydroxy-2H-1-benzopyran-2-one
	6,7-dihydroxycoumarin
	Aesculetin
	Cichorigenin
	Cichoriin aglucon
	Cichoriin aglycon
	Coumarin, 6,7-dihydroxy-
	Esculatin
	Esculetol
	Esculin aglucon
	Esculin aglycon
	NSC 26428
	asculetine
Inchi:	InChI=1S/C9H6O4/c10-6-3-5-1-2-9(12)13-8(5)4-7(6)11/h1-4,10-11H
InchiKey:	ILEDWLMCKZNDJK-UHFFFAOYSA-N
Formula:	C9H6O4
SMILES:	O=c1ccc2cc(O)c(O)cc2o1
Mol. weight [g/mol]:	178.14
CAS:	305-01-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.53		Crippen Method
logp	1.204		Crippen Method
mcvol	117.930	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Equilibrium partitioning of drug molecules between aqueous and amino acid ester-based ionic liquids:	https://www.doi.org/10.1016/j.jct.2013.02.011
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C305011&Units=SI

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