

Esculin

Other names:

2H-1-Benzopyran-2-one, 6-(«beta»-D-glucopyranosyloxy)-7-hydroxy-
6-(«beta»-D-Glucopyranosyloxy)-7-hydroxy-cumarin
Aesculin
Bicolorin
Crataegin
Enallachrome
Escosyl
Esculetin 6-«beta»-D-glucoside
Esculine
Esculoside
Polychrom
Polychrome
Vitamin C2
6-(«beta»-d-Glucopyranosyloxy)-7-hydroxy-2H-1-benzopyran-2-one
(-)-Esculin
7-Hydroxy-2-oxo-2h-chromen-6-yl hexopyranoside

Inchi:

InChI=1S/C15H16O9/c16-5-10-12(19)13(20)14(21)15(24-10)23-9-3-6-1-2-11(18)22-8(6)/4

InchiKey:

XHCADAYNFIFUHF-UHFFFAOYSA-N

Formula:

C15H16O9

SMILES:

O=c1ccc2cc(OC3OC(CO)C(O)C(O)C3O)c(O)cc2o1

Mol. weight [g/mol]:

340.28

CAS:

531-75-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.28		Crippen Method
logp	-1.323		Crippen Method
mcvol	220.960	ml/mol	McGowan Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C531759&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/63-987-7/Esculin.pdf>

Generated by Cheméo on 2024-04-19 19:46:00.948096535 +0000 UTC m=+15845209.868673850.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.