

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

Physical Properties

Property code	Value	Unit	Source
hf	-515.93	kJ/mol	Cheméo Relay (1.0)
ie	8.33	eV	Cheméo Relay (1.0)
log10ws	-1.82		Cheméo Relay (1.0)
logp	1.204		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
tb	626.00	K	Cheméo Relay (1.0)
tf	514.40	K	Cheméo Relay (1.0)

Sources

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>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C305011&Units=SI>
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):

Legend

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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