



Formula: C₁₀H₈O₅

MW: 208.17

CAS: 574-84-5

TNP NUMBER: TNP00177

MDL NUMBER: MFCD00006873

IUPAC: 7,8-dihydroxy-6-methoxycoumarin-2-one

Smiles: c1(c(c2c(cc1OC)ccc(o2)=O)O)O

SOURCE: Aglicon of Fraxin. Fraxin from bark of the common European ash ((Fraxinus Exelsior L.)

ACCEPTORS: 5

DONORS: 2

ROTATION BONDS: 3

N+O: 5

Chiral Centers: 0

LogP: 0.74

LogS: -2.71

LIPINSKI: 4

Monograph Number: 0004288

Title: Fraxetin

CAS Registry Number: 574-84-5

CAS Name: 7,8-Dihydroxy-6-methoxy-2H-1-benzopyran-2-one

Additional Names: 7,8-dihydroxy-6-methoxycoumarin

Molecular Formula: C₁₀H₈O₅

Molecular Weight: 208.17.

Percent Composition: C 57.70%, H 3.87%, O 38.43%

Literature References: The aglucon of fraxin. Obtained by heating fraxin with dil H₂SO₄.
Structure: Wessely, Demmer, Ber. 61, 1279 (1928). Synthesis: Aghoramurthy, Seshadri, J. Chem. Soc. 1954, 3065.

Properties: Plates from alc, mp 228. Turns yellow at 150 and brown at mp. Sol in 10 liters cold water, in 300 ml boiling water; somewhat more sol in alcohol; hardly sol in ether.

Melting point: mp 228

Derivative Type: Dimethyl ether

Additional Names: 6,7,8-Trimethoxycoumarin

Molecular Formula: C₁₂H₁₂O₅

Molecular Weight: 236.22.

Percent Composition: C 61.01%, H 5.12%, O 33.87%

Properties: Orthorhombic bipyramidal crystals, mp 104. bp_{0.2} 90-100.

Melting point: mp 104

Boiling point: bp0.2 90-100

Synonyms: 2H-1-Benzopyran-2-one,
7,8-dihydroxy-6-methoxy-;7,8-Dihydroxy-6-methoxy-2H-chromen-2-one;7,8-DIHYDROXY-6-ME
THOXYCOUMARIN;FRAXETIN;7,8-dihydroxy-6-methoxy-2-benzopyrone;Fratexin;7,8-Dihydrox
y-6-methoxy-2H-1-benzopyran-2-one;Fraccetain

CAS:574-84-5

MF:C10H8O5

MW:208.17

EINECS:209-376-2

Product Categories:Coumarins 7,8-DIHYDROXY-6-METHOXYCOUMARIN

Chemical Properties: mp 230-232C Merck 13,4288

CAS DataBase Reference: 574-84-5(

CAS DataBase Reference:) Xn Risk Statements 20/21/22-36/37/38 Safety Statements 26-36
7,8-DIHYDROXY-6-METHOXYCOUMARIN

Usage And Synthesis: 7,8-DIHYDROXY-6-METHOXYCOUMARIN

