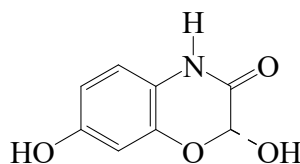




>>Entry Name: 2,7-Dihydroxy-2*H*-1,4-benzoxazin-3(4*H*)-one, 9Cl



CAS Registry Number: 69804-59-7

Molecular Formula: C₈H₇NO₄

Molecular Weight: 181.148

Accurate Mass: 181.037509

Percentage Composition: C 53.04%; H 3.89%; N 7.73%; O 35.33%

>>Variant: (*R*)-form

Molecular Formula: C₈H₇NO₄

Molecular Weight: 181.148

Accurate Mass: 181.037509

Percentage Composition: C 53.04%; H 3.89%; N 7.73%; O 35.33%

Biological Source: Identified in maize extracts

Solubility: Sol. MeOH, H₂O, CHCl₃

UV: [neutral] λ_{max} 254 (); 281 () (MeOH) (Berdy) [neutral] λ_{max} 253 (); 279 () (H₂O) (Berdy)

>>Derivative: 2-*O*-β-D-Glucopyranoside

Synonym(s): DHBOA-Glc

CAS Registry Number: 28512-70-1

Molecular Formula: C₁₄H₁₇NO₉

Molecular Weight: 343.29

Accurate Mass: 343.090334

Percentage Composition: C 48.98%; H 4.99%; N 4.08%; O 41.95%

Biological Source: Constit. of the roots of *Coix lachryma-jobi*

Physical Description: Cryst. (MeOH)

Melting Point: Mp 267-269°

Optical Rotation: [α]_D²⁴ +22.3 (c, 0.6 in Py)

UV: [neutral] λ_{max} 263 (log ε 4); 286 (sh) (log ε 3.84) (EtOH)

>>Derivative: 7-Me ether

Synonym(s): 2-Hydroxy-7-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one

CAS Registry Number: 17359-53-4

Molecular Formula: C₉H₉NO₄

Molecular Weight: 195.174

Accurate Mass: 195.053159

Percentage Composition: C 55.39%; H 4.65%; N 7.18%; O 32.79%

Biological Source: Constit. of *Coix lachryma-jobi*, wheat and maize

Physical Description: Cryst.

Melting Point: Mp 198-199.5°

UV: [neutral] λ_{max} 258 (log ε 4.06); 286 (sh) (log ε 3.78) (EtOH)

>>Derivative: 7-Me ether, 2-*O*-β-D-glucopyranoside

Synonym(s): HMBOA-Glc

CAS Registry Number: 17622-26-3

Molecular Formula: C₁₅H₁₉NO₉

Molecular Weight: 357.316

Accurate Mass: 357.105984

Percentage Composition: C 50.42%; H 5.36%; N 3.92%; O 40.30%

Biological Source: Constit. of the roots of *Coix lachryma-jobi* and *Aphelandra* spp.

Physical Description: Cryst. (MeOH)

Melting Point: Mp 250-251° (230-235°)

Optical Rotation: [α]_D²⁴ +31.4 (c, 0.8 in Py)

UV: [neutral] λ_{max} 205 (ε 12340); 259 (ε 9141); 282 (sh) (ε 7100) (MeOH)