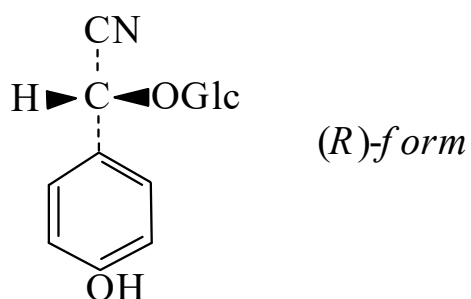




>>Entry Name: 2-(Glucopyranosyloxy)-2-(4-hydroxyphenyl)acetonitrile

ENTRY UNDER REVIEW

Synonym(s): α -(β -D-Glucopyranosyloxy)-4-hydroxybenzeneacetonitrile, 9Cl. *p*-Hydroxymandelonitrile β -D-glucoside



Molecular Formula: C₁₄H₁₇NO₇

Molecular Weight: 311.291

Accurate Mass: 311.100504

Percentage Composition: C 54.02%; H 5.50%; N 4.50%; O 35.98%

Use/Importance: Antineoplastic agent

Calculated Log P Data: Log P -2.6 (calc)

>>Variant: (2*R*)-form

Synonym(s): Taxiphyllin. **Phyllanthin**‡. **Phyllanthoside**‡

CAS Registry Number: 21401-21-8

Molecular Formula: C₁₄H₁₇NO₇

Molecular Weight: 311.291

Accurate Mass: 311.100504

Percentage Composition: C 54.02%; H 5.50%; N 4.50%; O 35.98%

Biological Source: Cyanogenic compd. of *Taxus* spp. and of bamboo (*Bambusa vulgaris*, Seaside arrow grass (*Triglochin maritima*) and *Bambusa guadua*). Also from *Stenocarpus sinuatus* and *Macadamia ternifolia*

Physical Description: Cryst. (EtOH/C₆H₆)

Melting Point: Mp 168-169°. Mp 176°

Optical Rotation: [α]_D²⁰ -667 (c, 0.37 in EtOH)

UV: [neutral] $\lambda_{\max}$ 216 (ϵ 17780); 222 (ϵ 15490); 277 (ϵ 21880) (MeOH) (Derep)

Other Data: Pharmacol. active isomer. Diastereoisomeric, not enantiomeric, with Dhurrin below

>>Variant: (2*S*)-form

Synonym(s): Dhurrin

CAS Registry Number: 499-20-7

Molecular Formula: C₁₄H₁₇NO₇

Molecular Weight: 311.291

Accurate Mass: 311.100504

Percentage Composition: C 54.02%; H 5.50%; N 4.50%; O 35.98%

Biological Source: Isol. from *Sorghum vulgare*

Use/Importance: Cyanogenic glucoside

Physical Description: Cryst. + 1H₂O (H₂O), cryst. + 1EtOH(EtOH)

Melting Point: Mp 165°

Solubility: BERDY SOL: Sol. MeOH, H₂O

UV: [neutral] $\lambda_{\max}$ 228 (ϵ 13000) (MeOH) (Berdy)

>>Derivative: 4'-Me ether

Synonym(s): 4'-*O*-Methyldhurrin

Molecular Formula: C₁₅H₁₉NO₇

Molecular Weight: 325.318

Accurate Mass: 325.116154

Percentage Composition: C 55.38%; H 5.89%; N 4.31%; O 34.43%

Biological Source: Occurs in bamboo

Melting Point: Mp 132°

Optical Rotation: [α]_D²⁰ -36 (c, 0.34 in 0.1% AcOH aq.)