



>>Derivative: 3-Me ether, nitrile
Synonym(s): 4-Cyano-2-methoxyphenol. Vanillonitrile

CAS Registry Number: 4421-08-3
Molecular Formula: $C_8H_7NO_2$
Molecular Weight: 149.149
Accurate Mass: 149.047679
Percentage Composition: C 64.42%; H 4.73%; N 9.39%; O 21.45%
Physical Description: Needles (H_2O)
Melting Point: Mp 89-90°
Aldrich: 16260-4

>>Derivative: 3-Me ether, 4-O- β -D-glucopyranoside

Molecular Formula: $C_{14}H_{18}O_9$
Molecular Weight: 330.291
Accurate Mass: 330.095085
Percentage Composition: C 50.91%; H 5.49%; O 43.60%
Biological Source: Isol. from fern *Vittaria flexuosa*. Thought to occur widely in plants
Physical Description: Needles (MeOH)
Melting Point: Mp 147-148° (143-146°)
Optical Rotation: $[\alpha]_D^{23}$ -82.6 (c, 0.5 in MeOH). $[\alpha]_D$ -62.7

>>Derivative: 3-Me ether, 4-O- β -D-glucopyranoside, β -D-glucopyranosyl ester
Synonym(s): Picrorhizin. Glucovanilloylglucose

CAS Registry Number: 60824-10-4

Molecular Formula: $C_{20}H_{28}O_{14}$
Molecular Weight: 492.433
Accurate Mass: 492.14791
Percentage Composition: C 48.78%; H 5.73%; O 45.49%
Biological Source: Isol. from *Abutilon indicum* and from rhizomes of *Picrorhiza kurrooa*
Melting Point: Mp 226-228°
Other Data: There seems to be some confusion about the application of the name Picrorhizin, which has also been applied to the monoglucosylated product above. The original ref. on Picrorhizin is inaccessible

>>Derivative: 3-Me ether, 4-O-(2-O-methyl- β -D-glucopyranoside)

Molecular Formula: $C_{15}H_{20}O_9$
Molecular Weight: 344.318
Accurate Mass: 344.110735
Percentage Composition: C 52.33%; H 5.85%; O 41.82%
Biological Source: Isol. from fern *Plagiogyria euphlebia*
Melting Point: Mp 223-225°
Optical Rotation: $[\alpha]_D$ -88.2

>>Derivative: 3-Me ether, 4-O-[4-hydroxy-3-methoxybenzoyl-($\rightarrow$ 6)- β -D-glucopyranoside]

Molecular Formula: $C_{22}H_{24}O_{12}$
Molecular Weight: 480.424
Accurate Mass: 480.12678
Percentage Composition: C 55.00%; H 5.04%; O 39.96%
Biological Source: Constit. of *Davallia mariesii*
Physical Description: Off-white solid
Optical Rotation: $[\alpha]_D^{22}$ -82.3 (c, 0.6 in MeOH)