



Molecular Formula: C₉H₁₁N₃O₂S

Molecular Weight: 225.271

Accurate Mass: 225.057197

Percentage Composition: C 47.99%; H 4.92%; N 18.65%; O 14.20%; S 14.23%

Use/Importance: Used as 8mM soln. in EtOAc for extraction-photometric detn. of Cu ($\lambda_{\max}$ 360 nm, ϵ 14000), Ni, Co, Ag

Physical Description: Cryst. (EtOH)

Solubility: Sol. EtOAc, EtOH, butanol

pKa Value: pK_{a1} 9.6; pK_{a2} 11.2

>>Derivative: Di-Ac

Molecular Formula: C₁₂H₁₂O₅

Molecular Weight: 236.224

Accurate Mass: 236.068475

Percentage Composition: C 61.02%; H 5.12%; O 33.86%

Melting Point: Mp 38°

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

Synonym(s): Bungeiside B. Cynanoneside B

CAS Registry Number: 149561-88-6

Molecular Formula: C₁₄H₁₈O₈

Molecular Weight: 314.291

Accurate Mass: 314.10017

Percentage Composition: C 53.50%; H 5.77%; O 40.73%

Biological Source: Constit. of *Cynanchum bungei* and *Cynanchum taiwanianum*

Physical Description: Amorph. powder

Optical Rotation: [α]_D -17.3 (c, 0.7 in MeOH)

>>Derivative: 4'-O-[β -D-Xylopyranosyl-(1 $\rightarrow$ 6)- β -D-glucopyranoside]

Synonym(s): Bungeiside D

CAS Registry Number: 149475-54-7

Molecular Formula: C₁₉H₂₆O₁₂

Molecular Weight: 446.407

Accurate Mass: 446.14243

Percentage Composition: C 51.12%; H 5.87%; O 43.01%

Biological Source: Constit. of *Cynanchum bungei*

Physical Description: Needles

Melting Point: Mp 238-240°

Optical Rotation: [α]_D -68.3 (c, 0.5 in MeOH)

>>Derivative: 2'-Me ether

Synonym(s): 4'-Hydroxy-2'-methoxyacetophenone, 8Cl. Isopeonol

CAS Registry Number: 493-33-4

Molecular Formula: C₉H₁₀O₃

Molecular Weight: 166.176

Accurate Mass: 166.062995

Percentage Composition: C 65.05%; H 6.07%; O 28.88%

Physical Description: Needles (H₂O)

Melting Point: Mp 139-140°