



>>Variant: Ergochrome BD

CAS Registry Number: 15140-37-1

Molecular Formula: $C_{32}H_{32}O_{15}$

Molecular Weight: 656.596

Accurate Mass: 656.174125

Percentage Composition: C 58.54%; H 4.91%; O 36.55%

Biological Source: Ergot pigment

Other Data: Acid $\rightarrow$ Ergochrome BC

>>Variant: Ergochrome BE

Synonym(s): Secalonic acid F

CAS Registry Number: 60687-07-2

Molecular Formula: $C_{32}H_{30}O_{14}$

Molecular Weight: 638.581

Accurate Mass: 638.16356

Percentage Composition: C 60.19%; H 4.74%; O 35.08%

Biological Source: Metab. of *Aspergillus aculeatus*

Physical Description: Yellow needles (C_6H_6 /cyclohexane)

Melting Point: Mp 218-221° (hot stage). Mp 253-256° (evacuated tube)

Optical Rotation: $[\alpha]_D^{20} +202$ (c, 0.13 in Py)

Solubility: BERDY SOL: Sol. bases, $CHCl_3$; poorly sol. H_2O

UV: [neutral] λ_{max} 236 (ϵ 19250); 263 (ϵ 17300); 338 (ϵ 37000) (EtOH) (Berdy) [neutral] λ_{max} 240 (ϵ 16980); 265 (ϵ 16980); 338 (ϵ 36300) (dioxan) (Berdy)

>>Variant: Ergochrome CC

Synonym(s): Ergoflavin

CAS Registry Number: 3101-51-7

Molecular Formula: $C_{30}H_{26}O_{14}$

Molecular Weight: 610.527

Accurate Mass: 610.13226

Percentage Composition: C 59.02%; H 4.29%; O 36.69%

Biological Source: Ergot pigment

Physical Description: Yellow needles (MeOH or dioxan)

Melting Point: Mp 350 dec.°

Optical Rotation: $[\alpha]_D^{11} +37.5$ (c, 1.236 in Me_2CO). $[\alpha]_D^{20} +105$ (Py)

UV: [neutral] λ_{max} 240 (ϵ 21380); 260 (ϵ 20900); 381 (ϵ 7940) (MeOH) (Berdy)

Other Data: λ_{max} 240 (log ϵ 4.33), 260 (4.32) and 381 nm (3.90)

>>Derivative: Hexa-Ac

Physical Description: Prisms ($CHCl_3$ /petrol)

Melting Point: Mp 248-249 dec.°

Optical Rotation: $[\alpha]_D +61.2$ (c, 0.62 in dioxan)

>>Variant: Ergochrome CD

CAS Registry Number: 15589-95-4

Molecular Formula: $C_{31}H_{30}O_{15}$

Molecular Weight: 642.569

Accurate Mass: 642.158475

Percentage Composition: C 57.95%; H 4.71%; O 37.35%

Biological Source: Ergot pigment

Other Data: Acid $\rightarrow$ Ergochrome CC