



CAS Registry Number: 164803-20-7

Molecular Formula: C₁₇H₂₄N₆O₈

Molecular Weight: 440.412

Accurate Mass: 440.165564

Percentage Composition: C 46.36%; H 5.49%; N 19.08%; O 29.06%

Biological Source: Prod. by *Chlorobium limicola f. thiosulfatophilum*

>>**Derivative:** 3-Me

Synonym(s): 2-Amino-6-(1,2-dihydroxypropyl)-3-methylpterin-4-one

CAS Registry Number: 111317-37-4

Molecular Formula: C₁₀H₁₃N₅O₃

Molecular Weight: 251.244

Accurate Mass: 251.10184

Percentage Composition: C 47.81%; H 5.22%; N 27.87%; O 19.10%

Biological Source: Isol. from the marine anthozoan *Astroides calycularis*

Physical Description: Pale yellow cryst. powder (MeOH)

Melting Point: Mp 229-231°

Optical Rotation: [α]_D -60 (c, 0.3 in 0.1M HCl)

Solubility: BERDY SOL: Sol. MeOH, H₂O

UV: [acid] $\lambda_{\max}$ 230 (ϵ 28200); 319 (ϵ 11700) (pH 1 H₂O) (Derep) [neutral] $\lambda_{\max}$ 242 (ϵ 28200); 276 (ϵ 24000); 356 (ϵ 9550) (H₂O pH 7) (Derep) [acid] $\lambda_{\max}$ 229 (ϵ 28183); 318 (ϵ 11750) (pH 1 buffer) (Berdy) [neutral] $\lambda_{\max}$ 242 (ϵ 28183); 275 (ϵ 23988); 356 (ϵ 9440) (pH 7 buffer) (Berdy)

>>**Derivative:** 7,8-Dihydro

Synonym(s): 7,8-Dihydrobiopterin

CAS Registry Number: 6779-87-9

Extra CAS Registry Numbers(s): 7644-44-2

Molecular Formula: C₉H₁₃N₅O₃

Molecular Weight: 239.233

Accurate Mass: 239.10184

Percentage Composition: C 45.19%; H 5.48%; N 29.27%; O 20.06%

Physical Description: Hygroscopic needles (H₂O or MeOH aq.)

Optical Rotation: [α]_D²² +35 (c, 0.4 in 0.1M NaOH)

>>**Derivative:** 5,6,7,8-Tetrahydro

see 5,6,7,8-Tetrahydrobiopterin, [LXF01-T](#)

>>**Variant:** (1'S,2'R)-form

Synonym(s): D-*erythro*-form

CAS Registry Number: 13039-62-8

Molecular Formula: C₉H₁₁N₅O₃

Molecular Weight: 237.218

Accurate Mass: 237.08619

Percentage Composition: C 45.57%; H 4.67%; N 29.52%; O 20.23%

Melting Point: Mp 300°

pKa Value: pK_{a2} 7.9

>>**Variant:** (1'S,2'S)-form

Synonym(s): L-*threo*-form. **Orinapterin.** Ciliapterin

CAS Registry Number: 13039-82-2

Molecular Formula: C₉H₁₁N₅O₃

Molecular Weight: 237.218

Accurate Mass: 237.08619

Percentage Composition: C 45.57%; H 4.67%; N 29.52%; O 20.23%

Biological Source: Isol. from human urine. Prod. by *Aphanizomenon flos-aquae*

Physical Description: Pale yellow cryst. (AcOH aq.)

Melting Point: Mp 300°

Optical Rotation: [α]_D +72 (0.1M HCl)

pKa Value: pK_{a2} 7.87