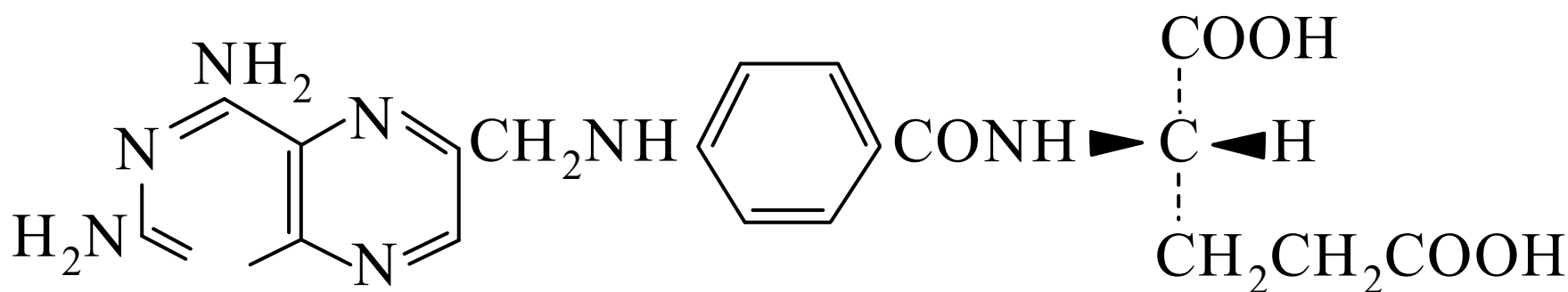




>>Entry Name: Aminopterin

Synonym(s): *N*-[4-[(2,4-Diamino-6-pteridiny)methyl]amino]benzoyl]glutamic acid, 9Cl. 4-Aminofolic acid. 4-Aminopteroylglutamic acid. Antifolic acid. Pteramina. APGA. NSC 739



CAS Registry Number: 54-62-6

Molecular Formula: C₁₉H₂₀N₈O₅

Molecular Weight: 440.418

Accurate Mass: 440.155667

Percentage Composition: C 51.82%; H 4.58%; N 25.44%; O 18.16%

Use/Importance: Antileukaemic factor and antagonist of Folic acid

Calculated Log P Data: Log P -1.65 (calc)

Hazard & Toxicity: LD₅₀ (mus, orl) 3 mg/kg. Human and exp. teratogenic effects

Aldrich: 86227-4

Fluka: 9328

Sigma: A1784

>>Variant: (*S*)-form

Synonym(s): L-form

Molecular Formula: C₁₉H₂₀N₈O₅

Molecular Weight: 440.418

Accurate Mass: 440.155667

Percentage Composition: C 51.82%; H 4.58%; N 25.44%; O 18.16%

Physical Description: Yellow cryst. (H₂O or NaHSO₃ aq.)

Melting Point: Mp 260-265 dec.°

Other Data: λ_{max} 370 nm, λ_{min} 333 nm (0.1*N* NaOH)

>>Derivative: Di-Na salt

Synonym(s): Aminopterin sodium, BAN, INN

CAS Registry Number: 58602-66-7

>>Derivative: Mg salt

Physical Description: Yellow cryst. + 2H₂O (H₂O)

>>Derivative: 4-*N*-Di-Me

Molecular Formula: C₂₁H₂₄N₈O₅

Molecular Weight: 468.471

Accurate Mass: 468.186967

Percentage Composition: C 53.84%; H 5.16%; N 23.92%; O 17.08%

Physical Description: Yellow cryst. (hydrate) (H₂O)

Melting Point: Mp 237-239 dec.°

>>Derivative: *N*-Me

References: