



>>Entry Name: (4-Aminobutyl)guanidine, 9CI

ENTRY UNDER REVIEW

Synonym(s): 4-Guanidinobutylamine. 1-Amino-4-guanidinobutane. **Agmatine**

CAS Registry Number: 306-60-5



Molecular Formula: C<sub>5</sub>H<sub>14</sub>N<sub>4</sub>

Molecular Weight: 130.192

Accurate Mass: 130.121846

Percentage Composition: C 46.13%; H 10.84%; N 43.03%

Biological Source: Present in ergot, pollen of *Ambrosia artemisiifolia* (Compositae), the sea anemone *Anthopleura japonica* and herring semen

Metabolism: Metabolic intermediate for polyamines. Synth. in mammalian brain

Biological Use/Importance: Endogenous neurotransmitter. Inhibits hyperalgesia and tolerance to morphine. NMDA receptor antagonist and nitric oxide synthase inhibitor

Melting Point: Mp 101.5-103°

>>Derivative: Sulfate

CAS Registry Number: 2482-00-0

Physical Description: Cryst.

Melting Point: Mp 229° (224-225°)

Aldrich: 10144-3

Fluka: 5083

Sigma: A7127

>>Derivative: *N*<sup>1</sup>-(4-Hydroxy-*E*-cinnamoyl)

Synonym(s): *N*<sup>1</sup>-*trans-p*-Coumaroylagmatine. 4-Hydroxycinnamoylagmatine

CAS Registry Number: 7295-86-5

Molecular Formula: C<sub>14</sub>H<sub>20</sub>N<sub>4</sub>O<sub>2</sub>

Molecular Weight: 276.338

Accurate Mass: 276.158626

Percentage Composition: C 60.85%; H 7.29%; N 20.27%; O 11.58%

(Gramineae)

Biological Use/Importance: Exhibits weak antifungal activity

Melting Point: Mp 215-217° (as picrate)

Solubility: BERDY SOL: Sol. H<sub>2</sub>O

UV: [neutral] λ<sub>max</sub> 229 (ε 33100); 300 (ε 26300) (H<sub>2</sub>O) (Berdy)

>>Derivative: *N*<sup>1</sup>-(4-Hydroxy-*Z*-cinnamoyl)

Synonym(s): *N*<sup>1</sup>-*cis-p*-Coumaroylagmatine

Molecular Formula: C<sub>14</sub>H<sub>20</sub>N<sub>4</sub>O<sub>2</sub>

Molecular Weight: 276.338

Accurate Mass: 276.158626

Percentage Composition: C 60.85%; H 7.29%; N 20.27%; O 11.58%

Biological Source: Constit. of *Albizzia julibrissin*

Biological Use/Importance: Leaf-opening factor

Physical Description: Syrup or powder

UV: [neutral] λ<sub>max</sub> 278 (ε 2000) (H<sub>2</sub>O)

>>Derivative: *N*<sup>1</sup>-(4-Hydroxy-3-methoxy-*E*-cinnamoyl)

Synonym(s): *N*<sup>1</sup>-*trans*-Feruloylagmatine

Molecular Formula: C<sub>15</sub>H<sub>22</sub>N<sub>4</sub>O<sub>3</sub>

Molecular Weight: 306.364

Accurate Mass: 306.169191

Percentage Composition: C 58.81%; H 7.24%; N 18.29%; O 15.67%

Biological Source: Isol. from *Triticum aestivum* exposed to low temps.

Biological Use/Importance: Antifungal agent