



>>Entry Name: Allophanic acid

Synonym(s): (Aminocarbonyl)carbamic acid, 9Cl. Ureidoformic acid. *N*-Carboxyurea. Carbamylcarbamic acid

CAS Registry Number: 625-78-5

$\text{H}_2\text{N}^4\text{CON}^2\text{HCOOH}$

Molecular Formula: $\text{C}_2\text{H}_4\text{N}_2\text{O}_3$

Molecular Weight: 104.065

Accurate Mass: 104.022193

Percentage Composition: C 23.08%; H 3.87%; N 26.92%; O 46.12%

General Statement: Not known in free state

Source/Synthesis: Isol. from *Butea monosperma* and *Echinops echinatus*

Other Data: Salts are unstable, being hydrol. to CO_2 , urea and carbonate by H_2O

>>Derivative: Mono-Na salt

CAS Registry Number: 26597-39-7

Physical Description: Solid

Other Data: Dec. above 150°

>>Derivative: Mono-K salt

CAS Registry Number: 26479-35-6

Physical Description: Solid

Other Data: Dec. above 150°

>>Derivative: Me ester

CAS Registry Number: 761-89-7

Molecular Formula: $\text{C}_3\text{H}_6\text{N}_2\text{O}_3$

Molecular Weight: 118.092

Accurate Mass: 118.037843

Percentage Composition: C 30.51%; H 5.12%; N 23.72%; O 40.64%

Physical Description: Needles (H_2O)

Melting Point: Mp 208 dec.°

Solubility: Sol. EtOH, hot H_2O

Rare Chemicals Library: S87617-8

>>Derivative: Et ester

CAS Registry Number: 626-36-8

Molecular Formula: $\text{C}_4\text{H}_8\text{N}_2\text{O}_3$

Molecular Weight: 132.119

Accurate Mass: 132.053493

Percentage Composition: C 36.36%; H 6.10%; N 21.20%; O 36.33%

Physical Description: Needles (H_2O)

Melting Point: Mp 195°

>>Derivative: Propyl ester

CAS Registry Number: 31598-83-1

Molecular Formula: $\text{C}_5\text{H}_{10}\text{N}_2\text{O}_3$

Molecular Weight: 146.146

Accurate Mass: 146.069143

Percentage Composition: C 41.09%; H 6.90%; N 19.17%; O 32.84%

Physical Description: Leaflets, needles (C_6H_6)

Melting Point: Mp $150\text{-}160^\circ$. Mp $179\text{-}180^\circ$

Solubility: Sol. hot H_2O