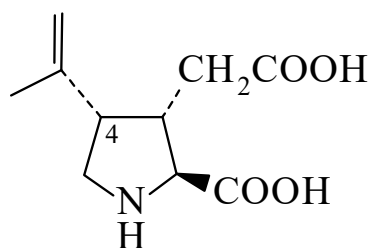




>>Entry Name: Kainic acid, INN

Synonym(s): 2-Carboxy-4-(1-methylethenyl)-3-pyrrolidineacetic acid, 9Cl. 3-Carboxymethyl-4-isopropenylproline. α -Kaininic acid. Digenic acid. Digenin



CAS Registry Number: 487-79-6

Related CAS Registry Numbers(s): 58002-62-3 92180-28-4 92180-29-5

Molecular Formula: $C_{10}H_{15}NO_4$

Molecular Weight: 213.233

Accurate Mass: 213.100109

Percentage Composition: C 56.33%; H 7.09%; N 6.57%; O 30.01%

Biological Source: Constit. of red algae *Digenea simplex* and *Centroceras clavulatum*

Use/Importance: Glutamate receptor agonist. Neurotoxin, formerly used as an anthelmintic agent

Physical Description: Cryst. + 1H₂O (EtOH aq.)

Melting Point: Mp 253-254 dec.°

Optical Rotation: $[\alpha]_D^{24}$ -14.8 (c, 1 in H₂O)

Solubility: BERDY SOL: Sol. H₂O

Calculated Log P Data: Log P -1.21 (calc)

UV: [neutral] $\lambda_{\max}$ 0 (end) (ϵ) (H₂O) (Derep)

Hazard & Toxicity: V. neurotoxic

Fluka: 60023

>>Derivative: N-Ac

CAS Registry Number: 59845-92-0

Melting Point: Mp 161-162°

Optical Rotation: $[\alpha]_D$ -53 (H₂O)

>>Derivative: Di-Me ester

CAS Registry Number: 4071-37-8

Boiling Point: Bp₄ 145°

Optical Rotation: $[\alpha]_D^{20}$ +23

>>Derivative: 4-Epimer

Synonym(s): α -Allokainic acid. α -Allokaininic acid

CAS Registry Number: 4071-39-0

Molecular Formula: $C_{10}H_{15}NO_4$

Molecular Weight: 213.233

Accurate Mass: 213.100109

Percentage Composition: C 56.33%; H 7.09%; N 6.57%; O 30.01%

Biological Source: Constit. of *Digenea simplex*

Melting Point: Mp 238-242 dec.°

Optical Rotation: $[\alpha]_D^{20}$ +7.7 (c, 1.3 in H₂O)

UV: [neutral] $\lambda_{\max}$ 0 (end) (ϵ) (H₂O) (Derep)

References: