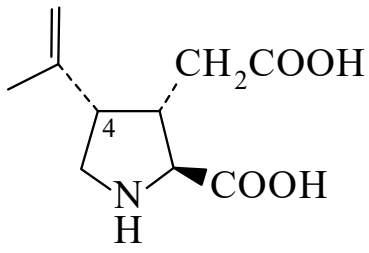
>>**Entry Name: Kainic acid,** INN

Synonym(s): 2-Carboxy-4-(1-methylethenyl)-3-pyrrolidineacetic acid, 9CI. 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. + $1H_2O$ (EtOH aq.)
Melting Point: Mp 253-254 dec.°
Optical Rotation: $[\alpha]_D^{24}$–14.8 (c, 1 in H_2O)
Solubility: BERDY SOL: Sol. H_2O
Calculated Log P Data: Log P –1.21 (calc)
UV: [neutral] λ_{max} 0 (end) (ε) (H_2O) (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 (H_2O)

>>**Derivative:** Di-Me ester

CAS Registry Number: 4071-37-8
Boiling Point: Bp_4 145°
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 H_2O)
UV: [neutral] λ_{max} 0 (end) (ε) (H_2O) (Derep)

References: