



CAS Registry Number: 554-35-8

Molecular Formula: $C_{10}H_{17}NO_6$

Molecular Weight: 247.247

Accurate Mass: 247.105589

Percentage Composition: C 48.58%; H 6.93%; N 5.67%; O 38.83%

Biological Source: Occurs in flax (*Linum usitatissimum*), manioc (*Manihot utilissimus*), *Phaseolus lunatus*, *Dimorphotheca Trifolium repens* and other plants. First isol. in 1830

Physical Description: Needles

Melting Point: Mp 143-144°

Optical Rotation: $[\alpha]_D -28.5$ (c, 3.86 in H_2O)

Hazard & Toxicity: Exp. teratogen

Sigma: L9131

>>Derivative: Nitrile, *O*-[β -D-glucopyranosyl-(1→6)- β -D-glucopyranoside]

Synonym(s): Linustatin. Linamarin gentiobioside

CAS Registry Number: 72229-40-4

Molecular Formula: $C_{16}H_{27}NO_{11}$

Molecular Weight: 409.389

Accurate Mass: 409.158414

Percentage Composition: C 46.94%; H 6.65%; N 3.42%; O 42.99%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 123-123.5°

Optical Rotation: $[\alpha]_D^{25} -37$ (c, 0.31 in H_2O)

>>Derivative: Ac

CAS Registry Number: 15805-98-8

Molecular Formula: $C_6H_{10}O_4$

Molecular Weight: 146.143

Accurate Mass: 146.05791

Percentage Composition: C 49.31%; H 6.90%; O 43.79%

Melting Point: Mp 61°

>>Derivative: Ac, bromide

Synonym(s): 2-Acetoxy-2-methylpropanoyl bromide. 1-(Bromocarbonyl)-1-methylethyl acetate

CAS Registry Number: 40635-67-4

Molecular Formula: $C_6H_9BrO_3$

Molecular Weight: 209.039

Accurate Mass: 207.993506

Percentage Composition: C 34.47%; H 4.34%; Br 38.22%; O 22.96%

Use/Importance: Reagent for deoxygenation of vicinal diols, and for synth. of nucleosides

Boiling Point: Bp₁₂ 75-77°

Density: d 1.43

Refractive Index: n_D^{20} 1.4530

>>Derivative: Ac, nitrile

CAS Registry Number: 56756-91-3

Molecular Formula: $C_6H_9NO_2$

Molecular Weight: 127.143

Accurate Mass: 127.063329

Percentage Composition: C 56.68%; H 7.13%; N 11.02%; O 25.17%

Boiling Point: Bp 180-182°

Rare Chemicals Library: S40331-8