



>>>Derivative: Heptyl ester

Synonym(s): Heptyl octanoate. Heptyl caprylate. FEMA 2553

CAS Registry Number: 2349-13-5

Molecular Formula: $C_{15}H_{30}O_2$

Molecular Weight: 242.401

Accurate Mass: 242.22458

Percentage Composition: C 74.33%; H 12.47%; O 13.20%

Use/Importance: Flavouring ingredient

Physical Description: Oil

Melting Point: $Mp -10^{\circ}$

Boiling Point: $Bp_{14} 160^{\circ}$

Density: $d^{30}_4 0.85$

Refractive Index: $n^{20}_D 1.4340$

>>>Derivative: Octyl ester

Synonym(s): Octyl octanoate. Capryl caprylate. FEMA 2811

CAS Registry Number: 2306-88-9

Molecular Formula: $C_{16}H_{32}O_2$

Molecular Weight: 256.428

Accurate Mass: 256.24023

Percentage Composition: C 74.94%; H 12.58%; O 12.48%

Biological Source: A minor component in the mandibular secretions of some species of bees and ants

Physical Description: Liq. with oily, fruity, sweet mildly green taste

Melting Point: $Mp -18.1^{\circ}$

Boiling Point: $Bp 306^{\circ}$. $Bp_{30} 192.5^{\circ}$

Density: $d^{25}_4 0.86$

Refractive Index: $n^{20}_D 1.4352$

>>>Derivative: 2-Propenyl ester

Synonym(s): 2-Propenyl octanoate. Allyl caprylate. FEMA 2037

CAS Registry Number: 4230-97-1

Molecular Formula: $C_{11}H_{20}O_2$

Molecular Weight: 184.278

Accurate Mass: 184.14633

Percentage Composition: C 71.70%; H 10.94%; O 17.36%

Use/Importance: Used in perfumery. Flavouring agent

Physical Description: Liq. with fruit-like aroma

Boiling Point: $Bp 222^{\circ}$. $Bp_{5.5} 87-88^{\circ}$

Density: $d^{30}_4 0.87$

Refractive Index: $n^{30}_D 1.4271$

>>>Derivative: Ph ester

Synonym(s): Phenyl octanoate. Phenyl caprylate

CAS Registry Number: 5457-78-3

Molecular Formula: $C_{14}H_{20}O_2$

Molecular Weight: 220.311

Accurate Mass: 220.14633

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

Physical Description: Oil

Boiling Point: $Bp_{10} 154^{\circ}$. $Bp_{0.3} 96-98^{\circ}$

>>>Derivative: 4-Methylphenyl ester

CAS Registry Number: 59558-23-5

Molecular Formula: $C_{15}H_{22}O_2$

Molecular Weight: 234.338

Accurate Mass: 234.16198

Percentage Composition: C 76.88%; H 9.46%; O 13.66%

Boiling Point: $Bp_{12} 175^{\circ}$

Density: $d^{24}_4 0.96$

Other: PB C26430