



>>Derivative: Benzoyl
Synonym(s): Hexyl benzoate. FEMA 3691

CAS Registry Number: 6789-88-4

Molecular Formula: $C_{13}H_{18}O_2$
Molecular Weight: 206.284
Accurate Mass: 206.13068
Percentage Composition: C 75.69%; H 8.79%; O 15.51%
Biological Source: Found in various fruits
Use/Importance: Flavouring ingredient
Physical Description: Apple-smelling liq.
Boiling Point: Bp 272°. Bp_{8.5} 138°
Aldrich: W36910-1
Supelco: 44-2681

>>Derivative: O-Sulfate

Molecular Formula: $C_6H_{14}O_4S$
Molecular Weight: 182.24
Accurate Mass: 182.06128
Percentage Composition: C 39.54%; H 7.74%; O 35.12%; S 17.60%
Biological Source: Isol. from the tunicate *Sidnyum turbinatum*
Physical Description: Amorph. solid (as Na salt)

>>Derivative: Propanoyl
Synonym(s): Hexyl propionate. FEMA 2576

CAS Registry Number: 2445-76-3

Molecular Formula: $C_9H_{18}O_2$
Molecular Weight: 158.24
Accurate Mass: 158.13068
Percentage Composition: C 68.31%; H 11.46%; O 20.22%
Physical Description: Liq.
Melting Point: Mp -57.5°
Boiling Point: Bp 185-186° (180°)
Density: d_4^{15} 0.87
Refractive Index: n_D^{25} 1.4067

>>Derivative: Butanoyl
Synonym(s): Hexyl butyrate

CAS Registry Number: 2639-63-6

Molecular Formula: $C_{10}H_{20}O_2$
Molecular Weight: 172.267
Accurate Mass: 172.14633
Percentage Composition: C 69.72%; H 11.70%; O 18.58%
Biological Source: Naturally occurring in many fruits
Physical Description: Liq.
Melting Point: Mp -78°
Boiling Point: Bp 207.8°
Density: d^{15} 0.87
Refractive Index: n_D^{20} 1.4170

References: