CAS Registry Number: 774-65-2
Molecular Formula: $C_{11}H_{14}O_2$
Molecular Weight: 178.23
Accurate Mass: 178.09938
Percentage Composition: C 74.13%; H 7.92%; O 17.95%
Boiling Point: Bp_2 96°

>>**Derivative:** Benzyl ester
Synonym(s): Benzyl benzoate, USAN**.** Ascabin. Benylate. Vanzoate. FEMA 2138. Many other names

CAS Registry Number: 120-51-4

Molecular Formula: $C_{14}H_{12}O_2$
Molecular Weight: 212.248
Accurate Mass: 212.08373
Percentage Composition: C 79.23%; H 5.70%; O 15.08%
Biological Source: Contained in Peru balsam and Tolu balsam. Isol. from other plants e.g. *Jasminum* spp., ylang-ylang oil
Use/Importance: Acaricide and pediculicide agent. Insect repellent component. Used in perfumery as fixative and in food flavouring, pharmaceutical excipient (solubilising agent, solvent)
Physical Description: Leaflets with balsamic/almond flavour and sharp, pungent flavour
Melting Point: Mp 21° (19.5°)
Boiling Point: Bp 323-324° (316-317°). $Bp_{0.1}$ 80-82°
Density: d^{18} 1.11
Calculated Log P Data: Log P 3.88 (uncertain value) (calc)
Other Data: Spar. steam-volatile
Hazard & Toxicity: Fl. p. 148°, autoignition temp. 480°. Eye, mucous membrane, and possible skin irritant. Hypersensitivity reactions reported. LD_{50} (rat, orl) 500 mg/kg

Aldrich: W21380-2
Fluka: 12390
Sigma: B6630

>>**Derivative:** Ph ester
see Phenyl benzoate, MTL19-R

>>**Derivative:** α-L-Rhamnopyranosyl ester
Synonym(s): Benzoyl α-L-rhamnopyranoside

Molecular Formula: $C_{13}H_{16}O_6$
Molecular Weight: 268.266
Accurate Mass: 268.09469
Percentage Composition: C 58.20%; H 6.01%; O 35.78%
Biological Source: Prod. by *Streptomyces griseoviridis*
Melting Point: Mp 145 dec.°
Optical Rotation: $[\alpha]_D^{20}$ –52 (c, 0.35 in MeOH)
UV: [neutral] λ_{max} 201 (log ε 4.02); 209 (log ε 3.51); 230 (log ε 4.11); 258 (log ε 2.83); 274 (log ε 2.98) (MeOH)

>>**Derivative:** Fluoride
Synonym(s): Benzoyl fluoride

CAS Registry Number: 455-32-3
Molecular Formula: C_7H_5FO
Molecular Weight: 124.114
Accurate Mass: 124.032443
Percentage Composition: C 67.74%; H 4.06%; F 15.31%; O 12.89%
Physical Description: Fuming liq.
Boiling Point: Bp 159-161°
Other Data: Hydrolysed by hot H_2O
Hazard & Toxicity: Highly irritant, causes burns, violent reaction with DMSO. Fl. p. 72/102°
Aldrich: 14074-0