



Molecular Formula: C₂₄H₃₈O₄

Molecular Weight: 390.562

Accurate Mass: 390.27701

Percentage Composition: C 73.81%; H 9.81%; O 16.39%

Biological Source: Reported as a natural product from heartwood of *Pterocarpus angolensis*, from *Penicillium olsonii* and from a *Streptomyces* sp. Almost certainly a contaminant (see note above)

Use/Importance: Important plasticiser. Environmental contamination reference chemical

Physical Description: Liq.

Melting Point: Mp -46°

Boiling Point: Bp₅ 231°

Solubility: Insol. H₂O

Density: d²⁰ 0.986

UV: [acid] λ_{max} 250 (ε); 283 (sh) (ε) (hexane) (Derep) [neutral] λ_{max} 275 (ε 1330) (isopropanol) (Derep)

Hazard & Toxicity: Mod. skin irritant. Low acute mammalian toxicity. Exp. hepatocarcinogen. Exp. reprod. and teratogenic effects. A non-genotoxic (exp.) carcinogen with weak peroxisome proliferating props.

Aldrich: D20115-4

Fluka: 80030

Sigma: P6699

Supelco: 4-8560

>>Derivative: Bis(2,5-dimethylhexyl) ester

Synonym(s): Bis(2,5-dimethylhexyl) phthalate. Phyllester

CAS Registry Number: 104719-70-2

Molecular Formula: C₂₄H₃₈O₄

Molecular Weight: 390.562

Accurate Mass: 390.27701

Percentage Composition: C 73.81%; H 9.81%; O 16.39%

Biological Source: Reported constit. of *Phyllanthus urinaria* and *Phyllanthus niruri* (see note above)

Melting Point: Mp 40°

>>Derivative: Dicyclohexyl ester

Synonym(s): Dicyclohexyl phthalate

CAS Registry Number: 84-61-7

Molecular Formula: C₂₀H₂₆O₄

Molecular Weight: 330.423

Accurate Mass: 330.18311

Percentage Composition: C 72.70%; H 7.93%; O 19.37%

Use/Importance: Plasticiser

Physical Description: Cryst.

Melting Point: Mp 64-66°

Boiling Point: Bp₁₀ 245-246°

Solubility: Insol. H₂O; sol. most org. solvs.

Density: d₂₀²⁰ 1.2

Aldrich: 30615-0

Fluka: 80110

Rare Chemicals Library: S60255-8

>>Derivative: Diheptyl ester

Synonym(s): Diheptyl phthalate

CAS Registry Number: 3648-21-3

Molecular Formula: C₂₂H₃₄O₄

Molecular Weight: 362.508

Accurate Mass: 362.24571

Percentage Composition: C 72.89%; H 9.45%; O 17.65%

Boiling Point: Bp₂₆ 264°

Density: d₄²⁰ 0.991

Refractive Index: n_D²⁰ 1.4867

Aldrich: 45481-8