



Biological Source: Metab. of *Penicillium bilaii*

Use/Importance: Plasticiser

Biological Use/Importance: Insect repellent. Now superseded

Melting Point: Mp -35°

Boiling Point: Bp 340°

Solubility: Insol. H_2O ; misc. common org. solvs.

Density: d_{20}^{20} 1.048

Refractive Index: n_D^{25} 1.4915

Hazard & Toxicity: Toxic, fl. p. 157° , autoignition temp. 400° . OES: long-term 5 mg m^{-3} ; short-term 10 mg m^{-3}

Aldrich: 24047-8

Fluka: 80100

Sigma: D2270

Supelco: R43-0680

>>**Derivative:** Butyl 2-ethylbutyl ester

Synonym(s): Butyl 2-ethylbutyl phthalate

CAS Registry Number: 26227-08-7

Molecular Formula: $C_{18}H_{26}O_4$

Molecular Weight: 306.401

Accurate Mass: 306.18311

Percentage Composition: C 70.56%; H 8.55%; O 20.89%

Biological Source: Constit. of *Oenanthe stolonifera*. Component of Shui Qin

Other Data: Claimed isolations of phthalate esters are suspect

>>**Derivative:** Dipentyl ester

Synonym(s): Dipentyl phthalate. Diamyl phthalate

CAS Registry Number: 131-18-0

Molecular Formula: $C_{18}H_{26}O_4$

Molecular Weight: 306.401

Accurate Mass: 306.18311

Percentage Composition: C 70.56%; H 8.55%; O 20.89%

Use/Importance: Plasticiser

Physical Description: Oily liq.

Melting Point: Mp -55°

Boiling Point: Bp 342° . Bp₁₁ $204-206^{\circ}$

Density: d^{20}_{20} 1.022

Refractive Index: n_D^{20} 1.4880

Fluka: 80154

>>**Derivative:** Dihexyl ester

Synonym(s): Dihexyl phthalate

CAS Registry Number: 84-75-3

Molecular Formula: $C_{20}H_{30}O_4$

Molecular Weight: 334.455

Accurate Mass: 334.21441

Percentage Composition: C 71.82%; H 9.04%; O 19.13%

Melting Point: Mp -40°

Boiling Point: Bp 333°

>>**Derivative:** Mono(2-ethylhexyl) ester

Synonym(s): Mono(2-ethylhexyl) phthalate

CAS Registry Number: 4376-20-9

Molecular Formula: $C_{16}H_{22}O_4$

Molecular Weight: 278.347

Accurate Mass: 278.15181

Percentage Composition: C 69.04%; H 7.97%; O 22.99%

Use/Importance: Active metab. of DEHP (see below)

Hazard & Toxicity: Potent eye irritant. Exp. hepatic and testicular effects