



>>Entry Name: Diethyl malonate

ENTRY UNDER REVIEW

Synonym(s): Diethyl propanedioate, 9CI. Malonic ester. Ethyl malonate. FEMA 2375

CAS Registry Number: 105-53-3



Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}_4$

Molecular Weight: 160.169

Accurate Mass: 160.07356

Percentage Composition: C 52.49%; H 7.55%; O 39.96%

Source/Synthesis: Produced by esterification of Propanedioic acid [DCG89-D](#) derived from cyanoacetic acid

Biological Source: Found in various fruits

Use/Importance: Important intermed. for manuf. of barbiturates etc. Synthetic reagent contg. active methylene group undergoing a wide range of condensations. Occasionally used as solvent. Flavour ingredient. Monomer for polyesters

Physical Description: Liq. with aromatic flavour

Melting Point: Mp -50°

Boiling Point: Bp 198.9° . Bp₂₀ 85°

Solubility: Sl. sol. H_2O ; sol. EtOH, Et₂O, CHCl_3 , C_6H_6

Density: d_4^{20} 1.055

Refractive Index: n_D^{20} 1.4143

Hazard & Toxicity: Low oral toxicity

Aldrich: W23750-7

Fluka: 63330

Sigma: M5629

>>Derivative: Na deriv

CAS Registry Number: 996-82-7

Molecular Formula: $\text{C}_7\text{H}_{11}\text{NaO}_4$

Molecular Weight: 182.151

Accurate Mass: 182.055502

Percentage Composition: C 46.16%; H 6.09%; Na 12.62%; O 35.13%

Physical Description: Needles (EtOH)

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 614B, (*ir*)

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Lux, H., *Ber.*, 1929, **62**, 1824, (*synth*)

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Large, R. *et al.*, *Org. Mass Spectrom.*, 1976, **11**, 582, (*ms*)

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Bauer, S.H. *et al.*, *J. Phys. Chem.*, 1983, **87**, 2411, (*cmr*)

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