



>>Entry Name: 2-Acetylpropanedioic acid, 9CI

Synonym(s): Acetylmalonic acid. Acetone-1,1-dicarboxylic acid



Molecular Formula: C₅H₆O₅

Molecular Weight: 146.099

Accurate Mass: 146.021525

Percentage Composition: C 41.11%; H 4.14%; O 54.76%

Other Data: Unstable

>>Derivative: Di-Et ester

CAS Registry Number: 570-08-1

Molecular Formula: C₉H₁₄O₅

Molecular Weight: 202.207

Accurate Mass: 202.084125

Percentage Composition: C 53.46%; H 6.98%; O 39.56%

Boiling Point: Bp₂₀ 125°

Solubility: Sol. dil. alkali

Refractive Index: n_D²⁰ 1.4471

Other Data: Exists as mixt. of keto and enol forms

>>Derivative: Di-Et ester, 2,4-dinitrophenylhydrazone

Melting Point: Mp 147°

>>Derivative: Di-Et ester, semicarbazone

Melting Point: Mp 106-107°

>>Derivative: Dinitrile

Synonym(s): Acetylmalononitrile

CAS Registry Number: 1187-11-7

Molecular Formula: C₅H₄N₂O

Molecular Weight: 108.099

Accurate Mass: 108.032363

Percentage Composition: C 55.56%; H 3.73%; N 25.91%; O 14.80%

Melting Point: Mp 138-141°

Aldrich: 36094-5

>>Derivative: Et ester-nitrile

Synonym(s): Ethyl 2-cyanoacetoacetate, 8CI. Ethyl 2-cyano-3-oxobutanoate, 9CI

CAS Registry Number: 634-55-9

Molecular Formula: C₇H₉NO₃

Molecular Weight: 155.153

Accurate Mass: 155.058244

Percentage Composition: C 54.19%; H 5.85%; N 9.03%; O 30.94%

Use/Importance: Used in photographic developers and processors

Physical Description: Needles with pungent odour

Melting Point: Mp 26°. Mp 185° (190°) (as semicarbazone)

Boiling Point: Bp₁₀ 102-104°

Solubility: Sol. EtOH, Et₂O, CHCl₃, CS₂, C₆H₆; spar. sol. H₂O giving an acid soln.

Density: d₄²⁰ 1.1107

Other Data: Dec. slowly on standing

References:

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Haller *et al.*, *Ann. Chim. (Paris)*, 1889, **17**, 204, (Et ester-nitrile)

Nef, J.U., *Annalen*, 1891, **266**, 105, (synth)

Isoshima, T., *Nippon Kagaku Zasshi*, 1956, **77**, 425, (Et ester-nitrile)

Tarbell, D.J. *et al.*, *J.O.C.*, 1957, **22**, 245, (synth)

Yasuda, H., *Yakugaku Zasshi*, 1959, **79**, 836, (Et ester-nitrile)

Burdett, J.L. *et al.*, *J. Phys. Chem.*, 1966, **70**, 939, (Et ester-nitrile)

Skarzewski, J., *Tetrahedron*, 1989, **45**, 4593, (synth, pmr)