



>>Entry Name: 2-Benzyl-3-oxobutanoic acid

ENTRY UNDER REVIEW

Synonym(s): 2-Benzylacetoacetic acid. 2-Acetyl-3-phenylpropanoic acid

CAS Registry Number: 2382-58-3

$\text{H}_3\text{CCOCH}(\text{COOH})\text{CH}_2\text{Ph}$

Molecular Formula: $\text{C}_{11}\text{H}_{12}\text{O}_3$

Molecular Weight: 192.214

Accurate Mass: 192.078645

Percentage Composition: C 68.74%; H 6.29%; O 24.97%

>>Variant: (±)-form

Molecular Formula: $\text{C}_{11}\text{H}_{12}\text{O}_3$

Molecular Weight: 192.214

Accurate Mass: 192.078645

Percentage Composition: C 68.74%; H 6.29%; O 24.97%

Physical Description: Oil with aromatic smell

Boiling Point: Bp_{13} 156-162°

Solubility: Spar. sol. H_2O

Other Data: Decarboxylates on warming

>>Derivative: Me ester

CAS Registry Number: 3666-82-8

Molecular Formula: $\text{C}_{12}\text{H}_{14}\text{O}_3$

Molecular Weight: 206.241

Accurate Mass: 206.094295

Percentage Composition: C 69.89%; H 6.84%; O 23.27%

Boiling Point: Bp_5 145°

>>Derivative: Et ester

Synonym(s): FEMA 2416

CAS Registry Number: 620-79-1

Molecular Formula: $\text{C}_{13}\text{H}_{16}\text{O}_3$

Molecular Weight: 220.268

Accurate Mass: 220.109945

Percentage Composition: C 70.89%; H 7.32%; O 21.79%

Boiling Point: Bp 276°

Solubility: Insol. H_2O , misc. EtOH, Et_2O

Density: d^{25} 1.061

Aldrich: W24160-1

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 280A, (*ir*)

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1216B, (*nmr*)

Ceresole, M., *Ber.*, 1882, **15**, 1871, (*synth*)

Rupe, H. *et al.*, *Annalen*, 1920, **426**, 33, (*resoln*)

Kabachnik, M.I. *et al.*, *Tetrahedron*, 1961, **12**, 76, (*ester*)

Kazankova, M.A. *et al.*, *Zh. Obshch. Khim.*, 1965, **35**, 1447, (*ester*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 214, (*Me ester*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 943, (*Me ester*)