



>>Entry Name: 3,3-Diphenylpropanoic acid

Synonym(s): β -Phenylbenzenepropanoic acid, 9Cl. 3,3-Diphenylpropionic acid, 8Cl. Benzhydrylic acid. β -Phenylhydrocinnamic acid

CAS Registry Number: 606-83-7

$\text{Ph}_2\text{CHCH}_2\text{COOH}$

Molecular Formula: $\text{C}_{15}\text{H}_{14}\text{O}_2$

Molecular Weight: 226.274

Accurate Mass: 226.09938

Percentage Composition: C 79.62%; H 6.24%; O 14.14%

Melting Point: Mp 157°

Aldrich: D21165-6

Fluka: 43220

>>Derivative: Me ester

CAS Registry Number: 23426-03-1

Molecular Formula: $\text{C}_{16}\text{H}_{16}\text{O}_2$

Molecular Weight: 240.301

Accurate Mass: 240.11503

Percentage Composition: C 79.97%; H 6.71%; O 13.32%

Melting Point: Mp 43-44°

Boiling Point: Bp₁ 148-150°

>>Derivative: Et ester

CAS Registry Number: 7476-18-8

Molecular Formula: $\text{C}_{17}\text{H}_{18}\text{O}_2$

Molecular Weight: 254.328

Accurate Mass: 254.13068

Percentage Composition: C 80.28%; H 7.13%; O 12.58%

Melting Point: Mp 22-23°

Boiling Point: Bp₁₂ 190-193°

>>Derivative: Amide

CAS Registry Number: 7474-19-3

Molecular Formula: $\text{C}_{15}\text{H}_{15}\text{NO}$

Molecular Weight: 225.29

Accurate Mass: 225.115364

Percentage Composition: C 79.97%; H 6.71%; N 6.22%; O 7.10%

Melting Point: Mp 125°

>>Derivative: Nitrile

Synonym(s): 2-Cyano-1,1-diphenylethane

CAS Registry Number: 2286-54-6

Molecular Formula: $\text{C}_{15}\text{H}_{13}\text{N}$

Molecular Weight: 207.274

Accurate Mass: 207.104799

Percentage Composition: C 86.92%; H 6.32%; N 6.76%

Melting Point: Mp 100°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 140A, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 986A, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1316C, (*ir*)

Wislicenus, W. *et al.*, *Ber.*, 1917, **50**, 250, (*synth*)

Mudzhoyan, A.L. *et al.*, *CA*, 1969, **71**, 60895w, (*synth*)

Elz, S. *et al.*, *J. Med. Chem.*, 2000, **43**, 1071-1084, (*nitrile*)