



>>Entry Name: 3,3,3-Triphenylpropanoic acid

Synonym(s): β,β -Diphenylbenzenepropanoic acid, 9Cl. 3,3-Diphenylhydrocinnamic acid

CAS Registry Number: 900-91-4

$\text{Ph}_3\text{CCH}_2\text{COOH}$

Molecular Formula: $\text{C}_{21}\text{H}_{18}\text{O}_2$

Molecular Weight: 302.372

Accurate Mass: 302.13068

Percentage Composition: C 83.42%; H 6.00%; O 10.58%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 177°

Aldrich: 25657-9

>>Derivative: Me ester

CAS Registry Number: 50354-49-9

Molecular Formula: $\text{C}_{22}\text{H}_{20}\text{O}_2$

Molecular Weight: 316.399

Accurate Mass: 316.14633

Percentage Composition: C 83.52%; H 6.37%; O 10.11%

Physical Description: Cryst. (C_6H_6)

Melting Point: Mp 120-121.5°

>>Derivative: Amide

Molecular Formula: $\text{C}_{21}\text{H}_{19}\text{NO}$

Molecular Weight: 301.387

Accurate Mass: 301.146664

Percentage Composition: C 83.69%; H 6.35%; N 4.65%; O 5.31%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 198°

>>Derivative: Chloride

CAS Registry Number: 33166-49-3

Molecular Formula: $\text{C}_{21}\text{H}_{17}\text{ClO}$

Molecular Weight: 320.817

Accurate Mass: 320.096792

Percentage Composition: C 78.62%; H 5.34%; Cl 11.05%; O 4.99%

Physical Description: Cryst.

Melting Point: Mp 132°

>>Derivative: Nitrile

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

Molecular Formula: $\text{C}_{21}\text{H}_{17}\text{N}$

Molecular Weight: 283.372

Accurate Mass: 283.136099

Percentage Composition: C 89.01%; H 6.05%; N 4.94%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 140°

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 986B, (*nmr*)

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

Boto, K.G. *et al.*, *Aust. J. Chem.*, 1973, **26**, 2409, (*synth*)