



>>Entry Name: 2,2-Diphenylpropanoic acid, 8Cl

Synonym(s):  $\alpha$ -Methyl- $\alpha$ -phenylbenzeneacetic acid, 9Cl.  $\alpha$ -Phenylhydratropic acid

CAS Registry Number: 5558-66-7

$\text{H}_3\text{CCPh}_2\text{COOH}$

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 177.5-178°

pKa Value:  $\text{p}K_{\text{a}1}$  5.77 (45% EtOH aq.)  $\text{p}K_{\text{a}1}$  7.2 (76% EtOH aq.)

Aldrich: D21160-5

>>Derivative: Me ester

CAS Registry Number: 50354-48-8

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%

Boiling Point: Bp<sub>3</sub> 149-152°

>>Derivative: Chloride

CAS Registry Number: 40997-78-2

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

Molecular Weight: 244.72

Accurate Mass: 244.065492

Percentage Composition: C 73.62%; H 5.35%; Cl 14.49%; O 6.54%

Melting Point: Mp 95-96°

>>Derivative: Amide

CAS Registry Number: 54561-74-9

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 149°

>>Derivative: Nitrile

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

CAS Registry Number: 5558-67-8

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%

Boiling Point: Bp<sub>2</sub> 145°

Aldrich: 12106-1

#### References:

*Aldrich Library of  $^{13}\text{C}$  and  $^1\text{H}$  FT NMR Spectra*, 1992, **2**, 985C; 1481C, (*nmr*)

*Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **2**, 139D; 425A, (*ir*)

Bateman, D.E. *et al.*, *J.A.C.S.*, 1927, **49**, 2914, (*synth*)

Steward, O.W. *et al.*, *J.C.S.(A)*, 1968, 3119, (*synth*)

Lu, M.C. *et al.*, *J. Med. Chem.*, 1987, **30**, 273, (*synth*, *nitrile*, *pmr*, *ir*)