



>>Entry Name: 2-Cyano-3,3-diphenyl-2-propenoic acid, 9CI

Synonym(s): 2-Cyano-3,3-diphenylacrylic acid, 8CI. Diphenylmethylenemalonic mononitrile. α -Cyano- β -phenylcinnamic acid

CAS Registry Number: 10380-41-3

$\text{Ph}_2\text{C}=\text{C}(\text{CN})\text{COOH}$

Molecular Formula: $\text{C}_{16}\text{H}_{11}\text{NO}_2$

Molecular Weight: 249.268

Accurate Mass: 249.078979

Percentage Composition: C 77.10%; H 4.45%; N 5.62%; O 12.84%

Physical Description: Needles (CHCl_3 /petrol)

Melting Point: Mp 178°

Other Data: Decarboxylates at 190°

>>Derivative: Et ester

Synonym(s): Etocrilene, INN. Etocrylene, USAN. Uvinul N35

CAS Registry Number: 5232-99-5

Molecular Formula: $\text{C}_{18}\text{H}_{15}\text{NO}_2$

Molecular Weight: 277.322

Accurate Mass: 277.110279

Percentage Composition: C 77.96%; H 5.45%; N 5.05%; O 11.54%

Use/Importance: UV screen, light stabiliser for polymers

Melting Point: Mp 95-97°

Boiling Point: Bp_{0.2} 174°

Calculated Log P Data: Log P 3.74 (calc)

Hazard & Toxicity: LD₅₀ (mus, ipr) 100 mg/kg

Aldrich: 41581-2

Rare Chemicals Library: S70151-3

>>Derivative: 2-Ethylhexyl ester

Synonym(s): Octocrilene, INN. Octocrylene, USAN. Uvinul N539

CAS Registry Number: 6197-30-4

Molecular Formula: $\text{C}_{24}\text{H}_{27}\text{NO}_2$

Molecular Weight: 361.483

Accurate Mass: 361.204179

Percentage Composition: C 79.74%; H 7.53%; N 3.87%; O 8.85%

Use/Importance: UV screen. Light stabiliser for polymers

Melting Point: Mp -10°

Boiling Point: Bp_{1.5} 218°

Density: d²⁰ 1.051

Refractive Index: n_D²⁰ 1.5670

Calculated Log P Data: Log P 6.79 (calc)

Aldrich: 41582-0

References:

Kohler, E.P. *et al.*, *Am. Chem. J.*, 1905, **33**, 333, (*synth*)

Cragoe, E.J. *et al.*, *J.O.C.*, 1950, **15**, 381, (*synth, ester*)

Belg. Pat., 1962, *General Aniline*, 619 809; *CA*, **58**, 13853, (*esters*)

Rivet-Le Guellac, P. *et al.*, *C. R. Hebd. Seances Acad. Sci.*, 1963, **257**, 2124, (*ir*)

Netherlands Pat., 1965, *General Aniline*, 293 502; *CA*, **64**, 4862a, (*synth, use*)

Rivet-Le Guellac, P. *et al.*, *J. Chim. Phys. Phys.-Chim. Biol.*, 1973, **70**, 1268, (*pmr*)

Odio, M.R. *et al.*, *Fundam. Appl. Toxicol.*, 1994, **22**, 355, (*octocrylene, tox*)

Odio, M.R. *et al.*, *Photodermatol. Photoimmunol. Photomed.*, 1994, **10**, 118, (*use*)

Martindale, The Extra Pharmacopoeia, 31st edn., *Pharmaceutical Press*, 1996, 1561, (*octocrylene*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., *Van Nostrand Reinhold*, 1992, DGX000