



Synonym(s): Fumaronitrile. (*E*)-1,2-Dicyanoethylene

CAS Registry Number: 764-42-1

Molecular Formula: C₄H₂N₂

Molecular Weight: 78.073

Accurate Mass: 78.021798

Percentage Composition: C 61.54%; H 2.58%; N 35.88%

Physical Description: Needles

Melting Point: Mp 96°

Boiling Point: Bp 186°

Solubility: Sol. EtOH, Et₂O, C₆H₆, H₂O, Me₂CO

Other Data: Q/e values for copolym., Q 0.29, e 2.73

Hazard & Toxicity: LD₅₀ (rat, orl) 132 mg/kg

Aldrich: 13101-6

Fluka: 47980

Sigma: F6759

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **1**, 502D; 644D; 645A; 695A; 742C; 844A, (*ir*)
- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **1**, 787B; 993B; 993C; 1119A; 1214A; 1360B, (*nmr*)
- Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 689C; 690A; 746A; 773B; 803D, (*ir*)
- Anschtütz, R., *Annalen*, 1928, **461**, 155, (*isom*)
- Golendeev, V.P., *J. Gen. Chem. USSR (Engl. Transl.)*, 1940, **10**, 1408, (*di-2-propenyl ester*)
- Justel, B., *Angew. Chem.*, 1943, **56**, 157, (*detn, Th*)
- Org. Synth., Coll. Vol.*, 2, 1943, 302, (*synth*)
- Welcher, F.J., *Organic Analytical Reagents*, Van Nostrand, New York, 1947, **2**, 41, (*synth, use*)
- Pressman, D. *et al.*, *J.A.C.S.*, 1948, **70**, 1352, (*synth, monoanilide*)
- Satta, V. *et al.*, *J.A.C.S.*, 1953, **75**, 4101, (*bis(2-ethylhexyl) ester*)
- Spatz, S.M. *et al.*, *J.O.C.*, 1958, **23**, 1559, (*monoester*)
- U.S. Pat.*, 1958, 2 848 366; *CA*, **52**, 19023e
- Klaban, J. *et al.*, *Coll. Czech. Chem. Comm.*, 1960, **25**, 2307, (*dihexyl ester*)
- Org. Synth., Coll. Vol.*, 4, 1963, 486, (*nitrile*)
- Sarvetnick, H.A., *Polyvinyl Chloride*, Van Nostrand Reinhold, 1969, 22, (*di-Et ester, copolym, reactivity ratios*)
- Devlin, C.J. *et al.*, *J.C.S. Perkin 1*, 1972, 1249, (*di-Et ester*)
- Benghiat, V. *et al.*, *J.C.S. Perkin 2*, 1972, 1758, (*cryst struct, monoamide*)
- Karrer, W. *et al.*, *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 849
- Junek, H. *et al.*, *Tetrahedron*, 1972, **28**, 4083, (*synth, pmr, deriv*)
- Morris, W.W., *J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037, (*ir*)
- Ito, A. *et al.*, *Org. Mass Spectrom.*, 1973, **7**, 1279, (*ms*)
- Kerr, R.O., *Benzene Its Ind. Deriv.*, Wiley, N.Y., 1975, (*rev*)
- Fieser and Fieser's Reagents for Organic Synthesis*, Wiley, 1975, **5**, 319
- Compton, D.A.C. *et al.*, *J.C.S. Perkin 2*, 1975, 400, (*ir, Raman, diesters*)
- Derissen, J.L., *J. Mol. Struct.*, 1977, **38**, 177, (*struct, ed*)
- Kirk-Othmer Encycl. Chem. Technol.*, 3rd edn., Wiley, 1978, **23**, 910, (*di-Et ester, copolym, reactivity ratios*)
- Greenley, R.Z., *J. Macromol. Sci., Chem., Part A*, 1980, **14**, 427, (*Q/e values*)
- Pfau, M. *et al.*, *Bull. Soc. Chim. Fr.*, Part II, 1982, 341, (*bis(dimethylamide)*)
- Ullmann's Encycl. Ind. Chem.*, 5th Ed., VCH, Weinheim, 1985, **A16**, 53, (*rev*)
- Encyclopaedia of Polymer Science and Engineering*, Wiley-Interscience, New York, 2nd edn., 1986, **4**, 779; 1987, **9**, 225
- Gutman, A.L. *et al.*, *Appl. Microbiol. Biotechnol.*, 1989, **32**, 11, (*mononitrile*)
- Gajiwski, J.J. *et al.*, *J.A.C.S.*, 1989, **111**, 9078, (*methyl β-cyanoacrylate, synth*)
- Kirk-Othmer Encycl. Chem. Technol.*, 4th edn., Wiley, 1991, **15**, 893, (*rev*)
- Merwin, L.H. *et al.*, *Magn. Reson. Chem.*, 1992, **30**, 440, (*cmr*)
- Handbook of Pharmaceutical Excipients*, 2nd edn., (eds. Wade, A. *et al.*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 197-198
- Narui, T. *et al.*, *Nat. Med. (Tokyo)*, 1995, **49**, 438-441, (*isobutylamide*)
- Martindale, The Extra Pharmacopoeia*, 31st edn., Pharmaceutical Press, 1996, 1086
- Encyclopedia of Food and Color Additives*, (ed. Burdock, G.A.), CRC Press, 1997, 1129-1131, (*props, use*)
- Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DEC600; FOU000; FOX000; FOY000; DSB600; DJJ800; DXD800