



>>Entry Name: Phenylacetylene

Synonym(s): Ethynylbenzene, 9Cl, 8Cl. Phenylethyne

CAS Registry Number: 536-74-3

PhC≡CH

Molecular Formula: C₈H₆

Molecular Weight: 102.135

Accurate Mass: 102.04695

Percentage Composition: C 94.08%; H 5.92%

Source/Synthesis: Found in coal tar

Use/Importance: Used as a 10% soln. in CH₂Cl₂ for extraction-photometric detn. of Pd ($\lambda_{\max}$ 317 nm)

Physical Description: Oil

Melting Point: Fp -45°

Boiling Point: Bp 142°. Bp₁₃ 35-36°

Solubility: Sol. Me₂CO, CHCl₃, C₆H₆, EtOH, Et₂O; insol. H₂O

Density: d^{12.5} 0.94

Refractive Index: n_D²⁰ 1.5490

Hazard & Toxicity: Flammable, fl. p. 31°. Polym. violently in presence of Pd(OAc)₂. Undergoes radical polym. Q/e values for copolym., Q 0.68, e 0.70

Aldrich: 11770-6

Fluka: 77840

Sigma: P6514

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 530C, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 946B, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1598B, (ir)

Normant, J., *Bull. Soc. Chim. Fr.*, 1963, 1868; 1888, (synth)

Org. Synth., Coll. Vol., 4, 1963, 763, (synth)

Ziegler, M. *et al.*, *Fresenius' Z. Anal. Chem.*, 1965, **210**, 344, (use)

Kaluza, F., *Chem. Ind. (London)*, 1967, 2045, (isol)

Kern, R.J., *J. Polym. Sci., Part A-1*, 1969, **7**, 621, (polym)

Hearn, M.T.W., *J. Magn. Reson.*, 1975, **19**, 401, (cmr)

Greenley, R.Z., *J. Macromol. Sci., Chem., Part A*, 1980, **14**, 427, (Q/e values)

Appling, J.R. *et al.*, *Org. Mass Spectrom.*, 1983, **18**, 282, (ms)

Császár, A.G. *et al.*, *J. Phys. Chem.*, 1989, **93**, 7644, (ir, Raman)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, PEB750

Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworths, 1990, 2727