



Synonym(s): Heptanedinitrile. 1,5-Dicyanopentane. Pimelonitrile

CAS Registry Number: 646-20-8

Molecular Formula: C₇H₁₀N₂

Molecular Weight: 122.169

Accurate Mass: 122.084398

Percentage Composition: C 68.82%; H 8.25%; N 22.93%

Melting Point: Mp -31.4°

Boiling Point: Bp₁₄ 175-176°

Solubility: Insol. H₂O; misc. EtOH, Et₂O, CHCl₃

Density: d¹⁸ 0.949

Refractive Index: n_D²⁰ 1.4472

Other Data: Solidifies to a glass

Hazard & Toxicity: LD₅₀ (mus, orl) 126 mg/kg

Aldrich: D7900-4

Fluka: 80530

Sigma: P6015

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 771C; 944A; 944B; 1357B, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 496A; 618C; 618D; 741C; 841D, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 582B; 643D; 644A; 801A, (ir)

Org. Synth., Coll. Vol., 2, 1943, 531; 535, (synth)

Corish, P.J. *et al.*, *J.C.S.*, 1958, 927, (esters)

Smiley, R.A. *et al.*, *J.O.C.*, 1960, **25**, 257, (nitrile)

Radell, J. *et al.*, *J. Phys. Chem.*, 1967, **71**, 1596, (cryst struct)

Angelo, B., *C. R. Hebd. Seances Acad. Sci.*, 1971, **273**, 1767, (synth)

Williamson, K.L. *et al.*, *J. Magn. Reson.*, 1978, **30**, 367, (cmr)

Marco, J.A. *et al.*, *Phytochemistry*, 1978, **17**, 1438, (occur)

Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **18**, 328, (rev, polyamides)

Newton, R.F. *et al.*, *J.C.S. Perkin 1*, 1980, 2346, (Me esters)

Bischoff, C. *et al.*, *J. Prakt. Chem.*, 1988, **330**, 379, (dihydrazide)

Harrison, A.G. *et al.*, *Org. Mass Spectrom.*, 1988, **23**, 723, (ms)

Ruholl, H. *et al.*, *Synthesis*, 1988, 54, (synth, pmr)

Bardet, L. *et al.*, *J. Raman Spectrosc.*, 1989, **20**, 41, (ir, Raman)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, HBD000; PIG000