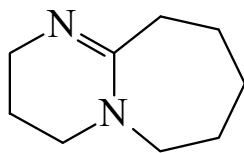




>>Entry Name: 2,3,4,6,7,8,9,10-Octahydropyrimido[1,2-*a*]azepine, 9CI

Synonym(s): 1,5-Diazabicyclo[5.4.0]undec-5-ene. DBU



CAS Registry Number: 6674-22-2

Molecular Formula: C₉H₁₆N₂

Molecular Weight: 152.239

Accurate Mass: 152.131348

Percentage Composition: C 71.01%; H 10.59%; N 18.40%

Use/Importance: Mild dehydrohalogenation reagent. Catalyst for Michael-type reactions and carboxylic acid esterification and a cocatalyst for 1-alkyne coupling reactions

Physical Description: Liq.

Boiling Point: Bp_{0.6} 80-83°

Density: d₄²⁰ 1.02

Aldrich: 13900-9

Fluka: 33482

Sigma: D2144

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1334C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 826B, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 794B, (*ir*)

Oediger, H. *et al.*, *Angew. Chem., Int. Ed.*, 1967, **6**, 76, (*synth*)

Oediger, H. *et al.*, *Synthesis*, 1972, 291, (*rev*)

Eiter, K. *et al.*, *Annalen*, 1978, 658, (*use*)

Ono, N. *et al.*, *Bull. Chem. Soc. Jpn.*, 1978, **51**, 2401, (*use*)

Hori, Y. *et al.*, *Chem. Lett.*, 1978, 73, (*use*)

Mukaiyama, T. *et al.*, *Chem. Lett.*, 1978, 461, (*use*)

Toda, T. *et al.*, *Chem. Lett.*, 1979, 171, (*use*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 141; **13**, 92; **16**, 105; **14**, 109; **15**, 109; **9**, 132; **11**, 155; **12**, 156; 479; **9**, 497, (*use*)

Wolkoff, P., *J.O.C.*, 1982, **47**, 1944, (*use*)