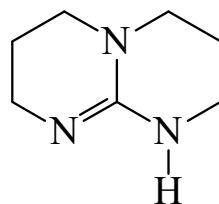




>>Entry Name: 1,3,4,6,7,8-Hexahydro-2*H*-pyrimido[1,2-*a*]pyrimidine, 9Cl

Synonym(s): 1,5,9-Triazabicyclo[4.4.0]dec-9-ene. TBD



CAS Registry Number: 5807-14-7

Molecular Formula: C₇H₁₃N₃

Molecular Weight: 139.2

Accurate Mass: 139.110947

Percentage Composition: C 60.40%; H 9.41%; N 30.19%

Use/Importance: Catalyst for a wide range of reactions

Melting Point: Mp 130-132°

Aldrich: 34557-1

Fluka: 90605

>>Derivative: Hydrobromide

CAS Registry Number: 74569-04-3

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 154°

>>Derivative: Picrate

CAS Registry Number: 74569-05-4

Physical Description: Cryst. (EtOH)

Melting Point: Mp 229-230° (220.5-222°)

Rare Chemicals Library: S89704-3

>>Derivative: *N*-Me

CAS Registry Number: 84030-20-6

Molecular Formula: C₈H₁₅N₃

Molecular Weight: 153.227

Accurate Mass: 153.126597

Percentage Composition: C 62.71%; H 9.87%; N 27.42%

Boiling Point: Bp_{0.1} 75-79°

Refractive Index: n_D²⁰ 1.3580

Aldrich: 35950-5

Fluka: 69440

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 595C, (*nmr*)

McKay, A.F. *et al.*, *Can. J. Chem.*, 1957, **35**, 1438, (*synth*)

Schmidtchen, F.P. *et al.*, *Chem. Ber.*, 1980, **113**, 2175, (*synth, pmr, cmr*)

Cheng, X. *et al.*, *Synth. Commun.*, 1993, **23**, 3191, (*synth*)