



>>Entry Name: (Cyano-C)trihydroborate(1-), 12Cl, 9Cl

CAS Registry Number: 33195-00-5

Related CAS Registry Numbers(s): 25895-62-9
[H₃BCN]⁽⁻⁾

Molecular Formula: CH₃BN⁽⁻⁾

Molecular Weight: 39.852

Accurate Mass: 40.035854

Percentage Composition: C 30.14%; H 7.59%; B 27.13%; N 35.15%

>>Derivative: Na salt

Synonym(s): Sodium cyanoborohydride

CAS Registry Number: 25895-60-7

Molecular Formula: CH₃BNNa

Molecular Weight: 62.842

Accurate Mass: 63.025621

Percentage Composition: C 19.11%; H 4.81%; B 17.20%; N 22.29%; Na 36.58%

Use/Importance: Commercially available either as solid or in soln. (THF or aq. NaOH). Mild reducing agent for org. functional groups, particularly for reductive amination of ketones

Physical Description: Cryst. (MeNO₂)

Melting Point: Mp 242 dec.°

Solubility: Sol. THF

Hazard & Toxicity: Severe poison, flammable solid

Aldrich: 29681-3

Fluka: 71435

Sigma: S8628

References:

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 1548B, (*ir*)

Berschied, J.R. *et al.*, *Inorg. Chem.*, 1970, **9**, 624; 1972, **11**, 930, (*ir*, *nmr*, *Raman*, *struct*)

Wade, R.C. *et al.*, *Inorg. Chem.*, 1970, **9**, 2146, (*synth*, *ir*, *nmr*)

Hall, L.W. *et al.*, *Inorg. Chem.*, 1975, **14**, 580, (*nmr*)

Nair, V. *et al.*, *J.O.C.*, 1978, **43**, 5013, (*use*, *Na salt*)

Hutchins, R.O. *et al.*, *Org. Prep. Proced. Int.*, 1979, **11**, 201, (*rev*, *use*)

Yamamoto, Y. *et al.*, *CA*, 1980, **92**, 139884j, (*synth*, *props*, *rev*)