



>>Entry Name: Aminopropanedinitrile, 9CI

Synonym(s): Aminomalonitrile

CAS Registry Number: 5181-05-5

$\text{H}_2\text{NCH}(\text{CN})_2$

Molecular Formula: $\text{C}_3\text{H}_3\text{N}_3$

Molecular Weight: 81.077

Accurate Mass: 81.032697

Percentage Composition: C 44.44%; H 3.73%; N 51.83%

General Statement: Free compd. not isol.

Use/Importance: Intermed. in polymerisation of HCN. Of interest as putative intermed. in prebiotic synth.

>>Derivative: 4-Methylbenzenesulfonyl

CAS Registry Number: 5098-14-6

Molecular Formula: $\text{C}_{10}\text{H}_9\text{N}_3\text{O}_2\text{S}$

Molecular Weight: 235.266

Accurate Mass: 235.041547

Percentage Composition: C 51.05%; H 3.86%; N 17.86%; O 13.60%; S 13.63%

Melting Point: Mp 180-181°

Aldrich: 22114-7

Fluka: 8370

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1598A

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 502B, (ir)

Ferris, J.P. *et al.*, *J.A.C.S.*, 1965, **87**, 4976; 1966, **88**, 3829

Org. Synth., 1968, **48**, 1, (synth)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 459, (use)

Freeman, F., *Synthesis*, 1981, 925, (rev)