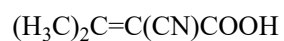




>>Entry Name: **2-Cyano-3-methyl-2-butenic acid**, 9CI

Synonym(s): 2-Cyano-3-methylcrotonic acid, 8CI. 2-Cyanosenecioic acid



Molecular Formula: C₆H₇NO₂

Molecular Weight: 125.127

Accurate Mass: 125.047679

Percentage Composition: C 57.59%; H 5.64%; N 11.19%; O 25.57%

General Statement: Mononitrile of (1-Methylethylidene)propanedioic acid [KNW46-O](#)

Physical Description: Plates (H₂O)

Melting Point: Mp 134-135°

>>Derivative: Me ester

Molecular Formula: C₇H₉NO₂

Molecular Weight: 139.154

Accurate Mass: 139.063329

Percentage Composition: C 60.42%; H 6.52%; N 10.07%; O 23.00%

Physical Description: Cryst.

Melting Point: Mp 20.3°

Boiling Point: Bp₃ 97°

Density: d₂₅²⁵ 1.06

Refractive Index: n_D²⁵ 1.4696

>>Derivative: Et ester

CAS Registry Number: 759-58-0

Molecular Formula: C₈H₁₁NO₂

Molecular Weight: 153.18

Accurate Mass: 153.078979

Percentage Composition: C 62.73%; H 7.24%; N 9.14%; O 20.89%

Physical Description: Needles (petrol)

Melting Point: Mp 33°

Boiling Point: Bp₁₈ 116-120°. Bp₁ 98-99°

Density: d 1.01

Refractive Index: n_D²⁰ 1.4640

Aldrich: 31058-1

>>Derivative: *tert*-Butyl ester

Molecular Formula: C₁₀H₁₅NO₂

Molecular Weight: 181.234

Accurate Mass: 181.110279

Percentage Composition: C 66.27%; H 8.34%; N 7.73%; O 17.66%

Physical Description: Cryst.

Melting Point: Mp 50°

Boiling Point: Bp₁₁ 111°

>>Derivative: Nitrile

see (1-Methylethylidene)propanedioic acid, [KNW46-O](#)

>>Derivative: Chloride

Molecular Formula: C₆H₆ClNO

Molecular Weight: 143.572

Accurate Mass: 143.013791

Percentage Composition: C 50.19%; H 4.21%; Cl 24.69%; N 9.76%; O 11.14%

Boiling Point: Bp₁₂ 106°

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Popp, F.D. *et al.*, *J.O.C.*, 1961, **26**, 2738, (*synth, Et ester*)

Eugster, C.M. *et al.*, *Helv. Chim. Acta*, 1963, **53**, 543, (*synth, ir*)

Torii, S. *et al.*, *Bull. Chem. Soc. Jpn.*, 1968, **41**, 2707, (*synth, pmr, ir*)

Texier-Boullet, F. *et al.*, *Tet. Lett.*, 1982, **23**, 4927, (*synth*)