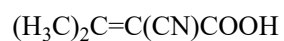




>>Entry Name: **2-Cyano-3-methyl-2-butenic acid**, 9CI

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



**Molecular Formula:** C<sub>6</sub>H<sub>7</sub>NO<sub>2</sub>

**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 (H<sub>2</sub>O)

**Melting Point:** Mp 134-135°

>>Derivative: Me ester

**Molecular Formula:** C<sub>7</sub>H<sub>9</sub>NO<sub>2</sub>

**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:** Bp<sub>3</sub> 97°

**Density:** d<sub>25</sub><sup>25</sup> 1.06

**Refractive Index:** n<sub>D</sub><sup>25</sup> 1.4696

>>Derivative: Et ester

**CAS Registry Number:** 759-58-0

**Molecular Formula:** C<sub>8</sub>H<sub>11</sub>NO<sub>2</sub>

**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:** Bp<sub>18</sub> 116-120°. Bp<sub>1</sub> 98-99°

**Density:** d 1.01

**Refractive Index:** n<sub>D</sub><sup>20</sup> 1.4640

**Aldrich:** 31058-1

>>Derivative: *tert*-Butyl ester

**Molecular Formula:** C<sub>10</sub>H<sub>15</sub>NO<sub>2</sub>

**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:** Bp<sub>11</sub> 111°

>>Derivative: Nitrile

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

>>Derivative: Chloride

**Molecular Formula:** C<sub>6</sub>H<sub>6</sub>ClNO

**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:** Bp<sub>12</sub> 106°

#### References:

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Warren, C.K. *et al.*, *J.C.S.*, 1958, 3972, (*synth, derivs*)

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*)