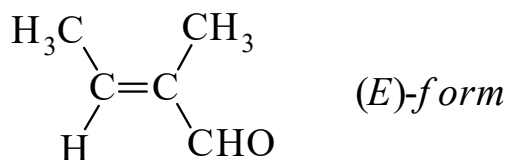




>>Entry Name: 2-Methyl-2-butenal, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2,3-Dimethylacrolein. 2-Methylcrotonaldehyde



CAS Registry Number: 1115-11-3

Molecular Formula: C<sub>5</sub>H<sub>8</sub>O

Molecular Weight: 84.118

Accurate Mass: 84.057515

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

>>Variant: (E)-form

Synonym(s): Tiglic aldehyde. Tiglaldehyde. FEMA 3407

CAS Registry Number: 497-03-0

Molecular Formula: C<sub>5</sub>H<sub>8</sub>O

Molecular Weight: 84.118

Accurate Mass: 84.057515

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Biological Source: Isol. from chives (*Allium schoenoprasum*)

Physical Description: Liq.

Boiling Point: Bp 116.5-117.5°. Bp<sub>119</sub> 63.2-65°

Solubility: Spar. sol. H<sub>2</sub>O

Density: d<sub>4</sub><sup>20</sup> 0.87

Refractive Index: n<sub>D</sub><sup>20</sup> 1.4475

Other Data: Readily oxidizes in air

Aldrich: W34070-7

Fluka: 89449

>>Derivative: Oxime

Molecular Formula: C<sub>5</sub>H<sub>9</sub>NO

Molecular Weight: 99.132

Accurate Mass: 99.068414

Percentage Composition: C 60.58%; H 9.15%; N 14.13%; O 16.14%

Physical Description: Cryst. (Et<sub>2</sub>O)

Melting Point: Mp 43°

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Red cryst. (EtOAc/Me<sub>2</sub>CO)

Melting Point: Mp 215.5-217.5° (222°)

>>Derivative: Semicarbazone

Physical Description: Needles (EtOH)

Melting Point: Mp 219° (234°)

>>Variant: (Z)-form

Synonym(s): Angelic aldehyde. Angelaldehyde

CAS Registry Number: 6038-09-1

Molecular Formula: C<sub>5</sub>H<sub>8</sub>O

Molecular Weight: 84.118

Accurate Mass: 84.057515

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Physical Description: Liq.

Other Data: Isom. to *E*-form after 2 weeks at r.t.

References: