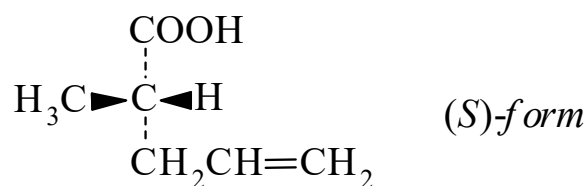




>>Entry Name: 2-Methyl-4-pentenoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Methylallylacetic acid. FEMA 3511



CAS Registry Number: 1575-74-2

Molecular Formula: C<sub>6</sub>H<sub>10</sub>O<sub>2</sub>

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

>>Variant: (S)-form

CAS Registry Number: 20626-61-3

Molecular Formula: C<sub>6</sub>H<sub>10</sub>O<sub>2</sub>

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Optical Rotation:  $[\alpha]_{\text{D}}^{25} +10.5$  (c, 1 in CHCl<sub>3</sub>)

>>Derivative: Me ester

Molecular Formula: C<sub>7</sub>H<sub>12</sub>O<sub>2</sub>

Molecular Weight: 128.171

Accurate Mass: 128.08373

Percentage Composition: C 65.60%; H 9.44%; O 24.97%

Optical Rotation:  $[\alpha]_{\text{D}}^{25} +17.38$  (neat)

>>Variant: (±)-form

Synonym(s): FEMA 3489

CAS Registry Number: 53729-46-7

Molecular Formula: C<sub>6</sub>H<sub>10</sub>O<sub>2</sub>

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Boiling Point: Bp 188-189°. Bp<sub>6</sub> 77-79°

Solubility: Sl. sol. H<sub>2</sub>O, misc. EtOH

Refractive Index:  $n_{\text{D}}^{20}$  1.4263

>>Derivative: Me ester

CAS Registry Number: 20459-96-5

Molecular Formula: C<sub>7</sub>H<sub>12</sub>O<sub>2</sub>

Molecular Weight: 128.171

Accurate Mass: 128.08373

Percentage Composition: C 65.60%; H 9.44%; O 24.97%

Boiling Point: Bp 137.5°

>>Derivative: Et ester

Synonym(s): FEMA 3489

CAS Registry Number: 53399-81-8

Extra CAS Registry Numbers(s): 105999-68-6

Molecular Formula: C<sub>8</sub>H<sub>14</sub>O<sub>2</sub>

Molecular Weight: 142.197

Accurate Mass: 142.09938

Percentage Composition: C 67.57%; H 9.92%; O 22.50%

Use/Importance: Flavouring agent

Boiling Point: Bp 153-155°

Solubility: Insol. H<sub>2</sub>O, misc. EtOH

Density: d 0.87

Refractive Index: n