



**Accurate Mass:** 154.09938  
**Percentage Composition:** C 70.10%; H 9.15%; O 20.75%  
**Use/Importance:** Preservative used in cosmetics

>>Derivative: Chloride

**CAS Registry Number:** 2614-88-2  
**Molecular Formula:** C<sub>6</sub>H<sub>7</sub>ClO  
**Molecular Weight:** 130.573  
**Accurate Mass:** 130.018542  
**Percentage Composition:** C 55.19%; H 5.40%; Cl 27.15%; O 12.25%  
**Boiling Point:** Bp<sub>12</sub> 69-71°. Bp<sub>16</sub> 78°

>>Derivative: Amide

**CAS Registry Number:** 16468-94-3  
**Molecular Formula:** C<sub>6</sub>H<sub>9</sub>NO  
**Molecular Weight:** 111.143  
**Accurate Mass:** 111.068414  
**Percentage Composition:** C 64.84%; H 8.16%; N 12.60%; O 14.40%  
**Physical Description:** Needles (H<sub>2</sub>O)  
**Melting Point:** Mp 172°

>>Derivative: Nitrile

**Synonym(s):** 1-Cyano-1,3-pentadiene

**CAS Registry Number:** 35684-10-7  
**Molecular Formula:** C<sub>6</sub>H<sub>7</sub>N  
**Molecular Weight:** 93.128  
**Accurate Mass:** 93.057849  
**Percentage Composition:** C 77.38%; H 7.58%; N 15.04%  
**Boiling Point:** Bp<sub>15</sub> 64-68°. Bp<sub>20</sub> 72°

>>Derivative: 2-Propenyl ester

**Synonym(s):** 2-Propenyl 2,4-hexadienoate. Allyl sorbate. FEMA 2041

**CAS Registry Number:** 7493-75-6

**Molecular Formula:** C<sub>9</sub>H<sub>12</sub>O<sub>2</sub>  
**Molecular Weight:** 152.193  
**Accurate Mass:** 152.08373  
**Percentage Composition:** C 71.03%; H 7.95%; O 21.03%  
**Use/Importance:** Flavouring ingredient

>>Variant: (2Z,4E)-form

**CAS Registry Number:** 5309-57-9  
**Molecular Formula:** C<sub>6</sub>H<sub>8</sub>O<sub>2</sub>  
**Molecular Weight:** 112.128  
**Accurate Mass:** 112.05243  
**Percentage Composition:** C 64.27%; H 7.19%; O 28.54%  
**Physical Description:** Needles (pentane)  
**Melting Point:** Mp 33-36°  
**Boiling Point:** Bp<sub>16</sub> 121-125°

>>Derivative: S-Benzylthiouronium salt

**Melting Point:** Mp 137°

>>Derivative: Me ester

**CAS Registry Number:** 6932-46-3  
**Boiling Point:** Bp<sub>11</sub> 60°. Bp<sub>21</sub> 80°