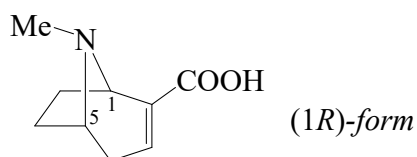




>>Entry Name: 8-Methyl-8-azabicyclo[3.2.1]oct-2-ene-2-carboxylic acid

Synonym(s): Anhydroecgonine. Ecgonidine



**Molecular Formula:** C<sub>9</sub>H<sub>13</sub>NO<sub>2</sub>

**Molecular Weight:** 167.207

**Accurate Mass:** 167.094629

**Percentage Composition:** C 64.65%; H 7.84%; N 8.38%; O 19.14%

**Biological Use/Importance:** Topical anaesthetic

**pKa Value:** p*K*<sub>a1</sub> 3.8; p*K*<sub>a2</sub> 9.8

>>Variant: (1*R*)-form

Synonym(s): (–)-form

**CAS Registry Number:** 484-93-5

**Molecular Formula:** C<sub>9</sub>H<sub>13</sub>NO<sub>2</sub>

**Molecular Weight:** 167.207

**Accurate Mass:** 167.094629

**Percentage Composition:** C 64.65%; H 7.84%; N 8.38%; O 19.14%

**Source/Synthesis:** Obt. semisynthetically from Cocaine

**Physical Description:** Cryst. (MeOH/EtOH)

**Melting Point:** Mp 235 dec.°

**Optical Rotation:** [α]<sub>D</sub><sup>14</sup> –84.6

>>Derivative: Hydrochloride

**CAS Registry Number:** 74242-55-0

**Physical Description:** Needles (EtOH) or tablets (H<sub>2</sub>O)

**Melting Point:** Mp 240-241°

**Optical Rotation:** [α]<sub>D</sub><sup>25</sup> –62.7 (H<sub>2</sub>O)

>>Derivative: Me ester

**CAS Registry Number:** 43021-26-7

**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%

**Boiling Point:** Bp<sub>7</sub> 107°

>>Derivative: Et ester

**CAS Registry Number:** 73045-45-1

**Molecular Formula:** C<sub>11</sub>H<sub>17</sub>NO<sub>2</sub>

**Molecular Weight:** 195.261

**Accurate Mass:** 195.125929

**Percentage Composition:** C 67.66%; H 8.78%; N 7.17%; O 16.39%

**Boiling Point:** Bp<sub>16</sub> 136-139°

**Solubility:** Sol. cold H<sub>2</sub>O, spar. sol. hot

>>Variant: (1*S*)-form

Synonym(s): (+)-form

**Molecular Formula:** C<sub>9</sub>H<sub>13</sub>NO<sub>2</sub>

**Molecular Weight:** 167.207

**Accurate Mass:** 167.094629

**Percentage Composition:** C 64.65%; H 7.84%; N 8.38%; O 19.14%

**Physical Description:** Cryst. + 1H<sub>2</sub>O (MeOH or MeOH/Et<sub>2</sub>O)

**Melting Point:** Mp 226-230°

**Solubility:** Sol. H<sub>2</sub>O; spar. sol. EtOH

>>Derivative: Me ester