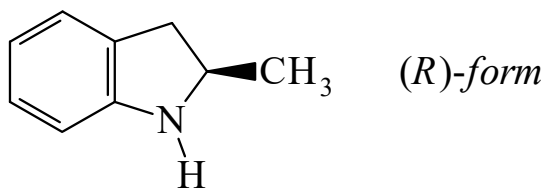




>>Entry Name: 2,3-Dihydro-2-methylindole, 9CI

Synonym(s): 2-Methylindoline



CAS Registry Number: 6872-06-6

Molecular Formula: C<sub>9</sub>H<sub>11</sub>N

Molecular Weight: 133.193

Accurate Mass: 133.089149

Percentage Composition: C 81.16%; H 8.32%; N 10.52%

Aldrich: M5160-1

>>Variant: (*R*)-form

CAS Registry Number: 22160-13-0

Molecular Formula: C<sub>9</sub>H<sub>11</sub>N

Molecular Weight: 133.193

Accurate Mass: 133.089149

Percentage Composition: C 81.16%; H 8.32%; N 10.52%

>>Derivative: *N*-Ac

Molecular Formula: C<sub>11</sub>H<sub>13</sub>NO

Molecular Weight: 175.23

Accurate Mass: 175.099714

Percentage Composition: C 75.40%; H 7.48%; N 7.99%; O 9.13%

Physical Description: Cryst. (petrol)

Melting Point: Mp 89°

Optical Rotation: [α]<sub>D</sub> +59.6 (EtOH)

>>Derivative: *N*-Benzoyl

Molecular Formula: C<sub>16</sub>H<sub>15</sub>NO

Molecular Weight: 237.301

Accurate Mass: 237.115364

Percentage Composition: C 80.98%; H 6.37%; N 5.90%; O 6.74%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 119°

Optical Rotation: [α]<sub>D</sub> +37 (EtOH)

>>Variant: (*S*)-form

CAS Registry Number: 22160-09-4

Molecular Formula: C<sub>9</sub>H<sub>11</sub>N

Molecular Weight: 133.193

Accurate Mass: 133.089149

Percentage Composition: C 81.16%; H 8.32%; N 10.52%

Physical Description: Liq. with blue fluor.

Boiling Point: Bp 228-229°

Optical Rotation: [α]<sub>D</sub> +7.2 (EtOH). [α]<sub>D</sub> -13.5 (Et<sub>2</sub>O). [α]<sub>D</sub> +8.3 (C<sub>6</sub>H<sub>6</sub>)

>>Derivative: Hydrochloride

Physical Description: Cryst. (C<sub>6</sub>H<sub>6</sub>)

Melting Point: Mp 58°

Optical Rotation: [α]<sub>D</sub> +1.7 (H<sub>2</sub>O)

>>Derivative: *N*-Ac

Physical Description: Cryst. (petrol)

Melting Point: Mp 89°

Optical Rotation: [α]<sub>D</sub> -61.9 (EtOH)