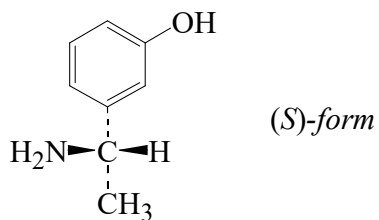




>>Entry Name: 3-(1-Aminoethyl)phenol, 9CI

Synonym(s): 1-(3-Hydroxyphenyl)ethylamine



CAS Registry Number: 63720-38-7

Related CAS Registry Numbers(s): 66033-00-9 66033-04-3 88196-70-7

Molecular Formula: C₈H₁₁NO

Molecular Weight: 137.181

Accurate Mass: 137.084064

Percentage Composition: C 70.04%; H 8.08%; N 10.21%; O 11.66%

>>Variant: (S)-form

CAS Registry Number: 123982-81-0

Molecular Formula: C₈H₁₁NO

Molecular Weight: 137.181

Accurate Mass: 137.084064

Percentage Composition: C 70.04%; H 8.08%; N 10.21%; O 11.66%

Optical Rotation: [α]_D -77.6 (c, 1 in MeOH) (>95% ee)

>>Derivative: Me ether

Synonym(s): 1-(3-Methoxyphenyl)ethylamine

CAS Registry Number: 82796-69-8

Molecular Formula: C₉H₁₃NO

Molecular Weight: 151.208

Accurate Mass: 151.099714

Percentage Composition: C 71.49%; H 8.67%; N 9.26%; O 10.58%

Optical Rotation: [α]_D -19.7 (c, 1 in MeOH) (>95% ee)

Other: Celgene 5351-00

>>Derivative: Benzyl ether

Molecular Formula: C₁₅H₁₇NO

Molecular Weight: 227.305

Accurate Mass: 227.131014

Percentage Composition: C 79.26%; H 7.54%; N 6.16%; O 7.04%

Optical Rotation: [α]_D²⁶ -2.56 (c, 1.05 in H₂O) (87.4% op)

>>Variant: (±)-form

Molecular Formula: C₈H₁₁NO

Molecular Weight: 137.181

Accurate Mass: 137.084064

Percentage Composition: C 70.04%; H 8.08%; N 10.21%; O 11.66%

Physical Description: Prisms (EtOH)

Melting Point: Mp 177-180°

>>Derivative: N-Chloroacetyl

CAS Registry Number: 53389-75-6

Molecular Formula: C₁₀H₁₂ClNO₂

Molecular Weight: 213.663

Accurate Mass: 213.055656

Percentage Composition: C 56.21%; H 5.66%; Cl 16.59%; N 6.56%; O 14.98%

Physical Description: Prisms (C₆H₆)

Melting Point: Mp 64.5-65.5°

References: