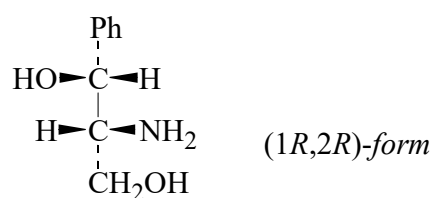




>>Entry Name: 2-Amino-1-phenyl-1,3-propanediol, 9Cl, 8Cl



CAS Registry Number: 3306-06-7

Related CAS Registry Numbers(s): 73473-94-6

Extra CAS Registry Numbers(s): 36391-67-0 36391-68-1 68534-64-5 105452-39-9 119364-52-2

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%

>>Variant: (1*R*,2*R*)-form

Synonym(s): (–)-*threo*-form

CAS Registry Number: 46032-98-8

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. (CHCl<sub>3</sub>)

Melting Point: Mp 115-117° (112-113°)

Optical Rotation: [α]<sub>D</sub><sup>20</sup> –26.7 (c, 1.0 in MeOH)

>>Derivative: *N,O*<sup>3</sup>-Di-Ac

Molecular Formula: C<sub>13</sub>H<sub>17</sub>NO<sub>4</sub>

Molecular Weight: 251.282

Accurate Mass: 251.115759

Percentage Composition: C 62.14%; H 6.82%; N 5.57%; O 25.47%

Physical Description: Cryst. (H<sub>3</sub>O)

Melting Point: Mp 121-122°

Optical Rotation: [α]<sub>D</sub> –6.7 (c, 4 in MeOH)

>>Derivative: *O*<sup>1</sup>,*O*<sup>3</sup>-Di-Ac

Molecular Formula: C<sub>13</sub>H<sub>17</sub>NO<sub>4</sub>

Molecular Weight: 251.282

Accurate Mass: 251.115759

Percentage Composition: C 62.14%; H 6.82%; N 5.57%; O 25.47%

Physical Description: Cryst. (MeOH/EtOAc) (as hydrochloride)

Melting Point: Mp 153.5-154.5° (hydrochloride)

Optical Rotation: [α]<sub>D</sub> –13.8 (c, 4 in MeOH)

>>Derivative: *N,O,O*-Tri-Ac

Molecular Formula: C<sub>15</sub>H<sub>19</sub>NO<sub>5</sub>

Molecular Weight: 293.319

Accurate Mass: 293.126324

Percentage Composition: C 61.42%; H 6.53%; N 4.78%; O 27.27%

Melting Point: Mp 93-95°

Optical Rotation: [α]<sub>D</sub> –28.5 (c, 3 in MeOH)

>>Derivative: *O*<sup>3</sup>-Me

Synonym(s): α-(1-Amino-2-methoxyethyl)benzenethanol. 2-Amino-3-methoxy-1-phenyl-1-propanol

CAS Registry Number: 51594-35-5

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%

Optical Rotation: [α]<sub>D</sub><sup>22</sup> –24.4 (c, 9.97 in CHCl<sub>3</sub>)