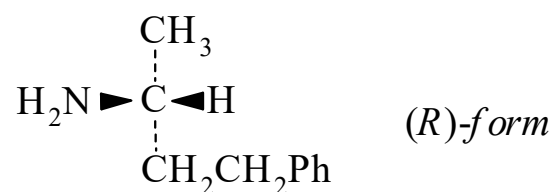




>>Entry Name: 4-Phenyl-2-butylamine

Synonym(s): α -Methylbenzenepropanamine, 9CI. 1-Methyl-3-phenylpropylamine, 8CI. 3-Amino-1-phenylbutane. γ -Aminobutylbenzene



CAS Registry Number: 22374-89-6

Molecular Formula: $\text{C}_{10}\text{H}_{15}\text{N}$

Molecular Weight: 149.235

Accurate Mass: 149.120449

Percentage Composition: C 80.48%; H 10.13%; N 9.39%

Aldrich: M7053-3

Fluka: 9200

Rare Chemicals Library: S40939-1

>>Variant: (R)-form

CAS Registry Number: 937-52-0

Molecular Formula: $\text{C}_{10}\text{H}_{15}\text{N}$

Molecular Weight: 149.235

Accurate Mass: 149.120449

Percentage Composition: C 80.48%; H 10.13%; N 9.39%

Optical Rotation: $[\alpha]_{\text{D}} -18$ (c, 1 in cyclohexane)

>>Derivative: Hydrochloride

CAS Registry Number: 826-16-4

Melting Point: Mp 114-115°

Optical Rotation: $[\alpha]_{\text{D}} +13$ (c, 1 in H_2O)

>>Derivative: N-Ac

CAS Registry Number: 22148-79-4

Molecular Formula: $\text{C}_{12}\text{H}_{17}\text{NO}$

Molecular Weight: 191.272

Accurate Mass: 191.131014

Percentage Composition: C 75.35%; H 8.96%; N 7.32%; O 8.36%

Melting Point: Mp 55°

Boiling Point: Bp₃ 142-150°

Optical Rotation: $[\alpha]_{\text{D}} -7.12$ (c, 0.7 in EtOH)

>>Derivative: N-Me

Molecular Formula: $\text{C}_{11}\text{H}_{17}\text{N}$

Molecular Weight: 163.262

Accurate Mass: 163.136099

Percentage Composition: C 80.93%; H 10.49%; N 8.58%

Optical Rotation: $[\alpha]_{\text{D}} -28$ (c, 2 in cyclohexane)

>>Derivative: N,N-Di-Me

CAS Registry Number: 35066-87-6

Molecular Formula: $\text{C}_{12}\text{H}_{19}\text{N}$

Molecular Weight: 177.289

Accurate Mass: 177.151749

Percentage Composition: C 81.30%; H 10.80%; N 7.90%

Optical Rotation: $[\alpha]_{\text{D}} -28$ (c, 2 in cyclohexane)