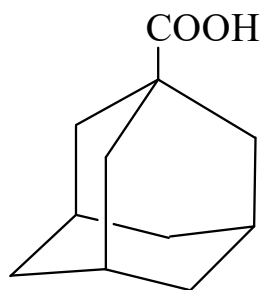




>>Entry Name: 1-Adamantanecarboxylic acid

Synonym(s): Tricyclo[3.3.1.1^{3,7}]decane-1-carboxylic acid, 9CI. Adamantoic acid



CAS Registry Number: 828-51-3

Molecular Formula: C₁₁H₁₆O₂

Molecular Weight: 180.246

Accurate Mass: 180.11503

Percentage Composition: C 73.30%; H 8.95%; O 17.75%

Physical Description: Cryst. (THF or MeOH)

Melting Point: Mp 254-255° (THF). Mp 180° (MeOH)

Aldrich: 10639-9

Fluka: 1823

Rare Chemicals Library: S15037-1

>>Derivative: Me ester

CAS Registry Number: 711-01-3

Molecular Formula: C₁₂H₁₈O₂

Molecular Weight: 194.273

Accurate Mass: 194.13068

Percentage Composition: C 74.19%; H 9.34%; O 16.47%

Melting Point: Mp 38-39°

>>Derivative: Chloride

CAS Registry Number: 2094-72-6

Molecular Formula: C₁₁H₁₅ClO

Molecular Weight: 198.692

Accurate Mass: 198.081142

Percentage Composition: C 66.50%; H 7.61%; Cl 17.84%; O 8.05%

Melting Point: Mp 49-51°

Hazard & Toxicity: Lachrymator

Aldrich: 11772-2

Fluka: 1820

>>Derivative: Amide

CAS Registry Number: 5511-18-2

Molecular Formula: C₁₁H₁₇NO

Molecular Weight: 179.261

Accurate Mass: 179.131014

Percentage Composition: C 73.70%; H 9.56%; N 7.81%; O 8.93%

Melting Point: Mp 188-190°

Aldrich: 39060-7

Rare Chemicals Library: S53467-6

>>Derivative: Nitrile

Synonym(s): 1-Cyanoadamantane

CAS Registry Number: 23074-42-2

Molecular Formula: C₁₁H₁₅N

Molecular Weight: 161.246

Accurate Mass: 161.120449

Percentage Composition: C 81.94%; H 9.38%; N 8.69%

Melting Point: Mp 185-190°

Aldrich: 13805-3

References: