



>>Entry Name: 3-Hydroxy-1-adamantanecarboxylic acid, 8Cl
Synonym(s): 3-Hydroxytricyclo[3.3.1.1^{3,7}]decane-1-carboxylic acid, 9Cl

CAS Registry Number: 42711-75-1

Molecular Formula: C₁₁H₁₆O₃
Molecular Weight: 196.246
Accurate Mass: 196.109945
Percentage Composition: C 67.32%; H 8.22%; O 24.46%
Physical Description: Cryst. (Me₂CO aq. or by subl.)
Melting Point: Mp 202-203°
pKa Value: pK_a 6.31 (25°) pK_a 6.42 (25°,50% EtOH aq.)

Rare Chemicals Library: S15023-1

>>Derivative: Me ester

CAS Registry Number: 68435-07-4
Molecular Formula: C₁₂H₁₈O₃
Molecular Weight: 210.272
Accurate Mass: 210.125595
Percentage Composition: C 68.55%; H 8.63%; O 22.83%
Physical Description: Cryst. (EtOH)
Melting Point: Mp 210-212.5°

>>Derivative: Et ester

Molecular Formula: C₁₃H₂₀O₃
Molecular Weight: 224.299
Accurate Mass: 224.141245
Percentage Composition: C 69.61%; H 8.99%; O 21.40%
Physical Description: Liq.

>>Derivative: Nitrile

Synonym(s): 3-Cyano-1-adamantanol

CAS Registry Number: 59223-70-0
Molecular Formula: C₁₁H₁₅NO
Molecular Weight: 177.246
Accurate Mass: 177.115364
Percentage Composition: C 74.54%; H 8.53%; N 7.90%; O 9.03%
Physical Description: Cryst. (pentane/CHCl₃)
Melting Point: Mp 209.5-211.5°

>>Derivative: Ac

CAS Registry Number: 42711-78-4
Molecular Formula: C₁₃H₁₈O₄
Molecular Weight: 238.283
Accurate Mass: 238.12051
Percentage Composition: C 65.53%; H 7.61%; O 26.86%
Physical Description: Cryst. (H₂O)
Melting Point: Mp 166-167°
pKa Value: pK_a 6.41 (25°,50% EtOH aq.)

>>Derivative: Me ether

Synonym(s): 3-Methoxy-1-adamantanecarboxylic acid

CAS Registry Number: 42711-80-8
Molecular Formula: C₁₂H₁₈O₃
Molecular Weight: 210.272
Accurate Mass: 210.125595
Percentage Composition: C 68.55%; H 8.63%; O 22.83%
Physical Description: Cryst. (cyclohexane)
Melting Point: Mp 126°
Boiling Point: Subl.₁₀ 110°
pKa Value: pK_a 6.45 (25°,50% EtOH aq.)