



>>Entry Name: 4-Oxo-1-adamantanecarboxylic acid

Synonym(s): 4-Oxotricyclo[3.3.1.1^{3,7}]decane-1-carboxylic acid, 9CI

CAS Registry Number: 56674-87-4

Molecular Formula: C₁₁H₁₄O₃

Molecular Weight: 194.23

Accurate Mass: 194.094295

Percentage Composition: C 68.02%; H 7.26%; O 24.71%

Physical Description: Cryst. (EtOAc/hexane)

Melting Point: Mp 171-172°

>>Derivative: Me ester

CAS Registry Number: 56674-88-5

Molecular Formula: C₁₂H₁₆O₃

Molecular Weight: 208.257

Accurate Mass: 208.109945

Percentage Composition: C 69.21%; H 7.74%; O 23.05%

Physical Description: Cryst. (hexane)

Melting Point: Mp 53-54°

Rare Chemicals Library: S2569-1

>>Derivative: Me ester, oxime

CAS Registry Number: 56674-89-6

Molecular Formula: C₁₂H₁₇NO₃

Molecular Weight: 223.271

Accurate Mass: 223.120844

Percentage Composition: C 64.55%; H 7.67%; N 6.27%; O 21.50%

Physical Description: Cryst. (hexane)

Melting Point: Mp 99-101°

References:

Lantvoev, V.I., *Zh. Org. Khim.*, 1975, **11**, 1567; *J. Org. Chem. USSR (Engl. Transl.)*, 1546, (synth, pmr, ir)

Manchand, P.S. *et al.*, *J. Med. Chem.*, 1990, **33**, 1992, (synth, pmr, ir, cmr)