



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:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 538C; 745B; 846C, (*ir*)

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **1**, 838A; 1364A, (*nmr*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 15

Stetter, H. *et al.*, *Chem. Ber.*, 1970, **103**, 863, (*synth*)

Goh, S.H. *et al.*, *J. Organomet. Chem.*, 1972, **43**, 401, (*nitrile*)

Maciel, G.E. *et al.*, *Org. Magn. Reson.*, 1974, **6**, 178, (*cmr*)

Ridyard, C.H. *et al.*, *J.C.S. Perkin 2*, 1996, 1811-1819, (*Me ester, synth, ir, pmr, cmr*)