



CAS Registry Number: 39716-58-0
Molecular Formula: C₅H₇ClO
Molecular Weight: 118.562
Accurate Mass: 118.018542
Percentage Composition: C 50.65%; H 5.95%; Cl 29.90%; O 13.49%
Physical Description: Liq.
Boiling Point: Bp 128°
Aldrich: 46847-9

>>Derivative: Amide

CAS Registry Number: 6852-94-4
Molecular Formula: C₅H₉NO
Molecular Weight: 99.132
Accurate Mass: 99.068414
Percentage Composition: C 60.58%; H 9.15%; N 14.13%; O 16.14%
Physical Description: Cryst. (toluene)
Melting Point: Mp 104.5-105.5° (94°)
Boiling Point: Bp 230°. Subl._{0.1} 80°

>>Derivative: Nitrile

Synonym(s): 4-Cyano-1-propene. Allylacetonitrile

CAS Registry Number: 592-51-8
Molecular Formula: C₅H₇N
Molecular Weight: 81.117
Accurate Mass: 81.057849
Percentage Composition: C 74.04%; H 8.70%; N 17.27%
Physical Description: Liq.
Boiling Point: Bp 140°. Bp₄₀ 60-61°
Solubility: Insol. H₂O; misc. EtOH, Et₂O
Density: d²⁴ 0.824
Refractive Index: n_D¹⁴ 1.4213

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 499B, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 778A, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 584A, (*ir*)
Sadtler Standard NMR Spectra, 14093, (*pmr*)
Fittig, R. *et al.*, *Annalen*, 1881, **208**, 37, (*synth*)
Croxall, W.J. *et al.*, *J.A.C.S.*, 1950, **72**, 803-808, (*2-propenyl ester*)
Ragazzini, M. *et al.*, *Eur. Polym. J.*, 1970, **6**, 1331, (*amide*)
Ireland, R.E. *et al.*, *J.A.C.S.*, 1976, **98**, 2868, (*synth*)
Eisch, J.J. *et al.*, *J.A.C.S.*, 1979, **101**, 1148, (*synth*)
Günther, H.J. *et al.*, *Annalen*, 1984, 15, (*synth, cmr*)
Maillard, B. *et al.*, *Nouv. J. Chim.*, 1987, **11**, 7, (*esters, synth*)
Glover, S.A. *et al.*, *Aust. J. Chem.*, 1993, **46**, 1213, (*nitrile*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 640
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2119-2120
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, PBQ750