



Use/Importance: Flavouring ingredient

Boiling Point: Bp 153°

>>**Derivative:** Chloride

CAS Registry Number: 5238-27-7

Molecular Formula: C₆H₁₁ClO

Molecular Weight: 134.605

Accurate Mass: 134.049842

Percentage Composition: C 53.54%; H 8.24%; Cl 26.34%; O 11.89%

Boiling Point: Bp 140-140.8°

>>**Derivative:** Amide

CAS Registry Number: 6941-49-7

Molecular Formula: C₆H₁₃NO

Molecular Weight: 115.175

Accurate Mass: 115.099714

Percentage Composition: C 62.57%; H 11.38%; N 12.16%; O 13.89%

Melting Point: Mp 79.6°

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **1**, 761C, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 579D, (*ir*)
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 288A, (*ir*)
Ställberg-Sterhagen, S., *Ark. Kemi*, No. 15, 1947, **23A**, (*abs config*)
Smith, L.I. *et al.*, *J.A.C.S.*, 1957, **79**, 2962, (*synth*)
Falbe, J. *et al.*, *Chem. Ber.*, 1964, **97**, 3088, (*synth*)
Goering, H.L. *et al.*, *J.A.C.S.*, 1965, **87**, 1748, (*abs config*)
White, D.R. *et al.*, *Chem. Comm.*, 1974, 988, (*synth*)
Riley, R.G. *et al.*, *Tetrahedron*, 1974, **30**, 1171, (*synth*)
Meyers, A.I. *et al.*, *J.A.C.S.*, 1976, **98**, 567, (*synth*)
Helmchen, G. *et al.*, *Angew. Chem., Int. Ed.*, 1979, **18**, 63, (*synth*)
Opdyke, D.L.J., *Food Chem. Toxicol.*, 1982, **20**, 763, (*rev, tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 250; 525; 582
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1009-1010; 1798-1799; 1882-1883
de Jesus, P.C. *et al.*, *Synth. Commun.*, 1998, **28**, 2893-2901, (*resoln*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4921
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MQJ750