



SIGMA-ALDRICH

3050 Spruce Street
Saint Louis, Missouri 63103 USA
Telephone 800-325-5832 • (314) 771-5765
Fax (314) 286-7828
email: techserv@sial.com
sigma-aldrich.com

Product Information

Acetonitrile ACS Reagent Grade

Product Number **36,045-7**
Store at Room Temperature

Exact replacement for Product Number A 6914

Product Description

Molecular Formula: C₂H₃N
Molecular Weight: 41.05
CAS Number: 75-05-8
Boiling Point: 81.6 °C¹
Density: 0.787 g/ml (15 °C)¹
Surface tension: 29.04 dynes/cm (20 °C)¹
Synonyms: methyl cyanide, cyanomethane, ethanenitrile¹

This product is designated as ACS Reagent grade, and meets the specifications of the American Chemical Society (ACS) for reagent chemicals.

Acetonitrile is a widely used, polar aprotic organic solvent. Acetonitrile is utilized as a starting material for the production of such compounds as acetophenone, α -naphthaleneacetic acid, thiamine, and acetamidine. It can be used in the recrystallization of steroids and as a solvent for non-aqueous titrations, as well as a non-aqueous solvent for inorganic salts.¹ In analytical chemistry, acetonitrile is utilized in such areas as biopartitioning studies, in the HPLC analysis of small organic compounds, and enantiomer resolution by LC on polysaccharide type chiral stationary phases.^{2,3,4}

A method for the pre-fractionation of lysates of cells and tissue for proteomics analysis that incorporates a five-step gradient of increasing acetonitrile concentrations has been published.⁵ A protocol has been reported for the enrichment of low-abundance peptides for proteomic analysis that uses acetonitrile as part of the elution-modified displacement chromatography method.⁶ A method that incorporates acetonitrile in the mobile phase for the LC/ESI-MS analysis of flavonoid glycosides has been described.⁷ The use of acetonitrile and other organic solvents in mixed organic/aqueous solvents in the digestion of proteins on immobilized trypsin columns has been reported.⁸

Acetonitrile has been used in the synthesis of such organic compounds as functionalized pyrrolo[3,2-d]pyrimidines, methanesulfonyl carbonates, and arylzinc compounds.^{9,10,11} Inorganic compounds which have been synthesized in acetonitrile include dimorphic copper(I) coordination polymers, osmium phosphiniminato complexes, and vanadium iron sulfur clusters as structural analogs to the PN cluster of nitrogenase.^{12,13,14}

Precautions and Disclaimer

For Laboratory Use Only. Not for drug, household or other uses.

Preparation Instructions

This product is miscible in water, methanol, ethyl acetate, acetone, ether, chloroform, and many unsaturated hydrocarbons.¹

References

1. The Merck Index, 12th ed., Entry# 68.
2. Cimpean, D. M., and Poole, C. F., Systematic search for surrogate chromatographic models of biopartitioning processes. *Analyst*, **127(6)**, 724-729 (2002).
3. Loregian, A., et al., Separation methods for acyclovir and related antiviral compounds. *J. Chromatogr. B Biomed. Sci. Appl.*, **764(1-2)**, 289-311 (2001).
4. Tachibana, K., and Ohnishi, A., Reversed-phase liquid chromatographic separation of enantiomers on polysaccharide type chiral stationary phases. *J. Chromatogr. A*, **906(1-2)**, 127-154 (2001).
5. Badock, V., et al., Prefractionation of protein samples for proteome analysis using reversed-phase high-performance liquid chromatography. *Electrophoresis*, **22(14)**, 2856-2864 (2001).
6. Wilkins, J. A., et al., Selective enrichment of low-abundance peptides in complex mixtures by elution-modified displacement chromatography and their identification by electrospray ionization mass spectrometry. *Anal. Chem.*, **74(16)**, 3933-3941 (2002).

7. Cuyckens, F., and Claeys, M., Optimization of a liquid chromatography method based on simultaneous electrospray ionization mass spectrometric and ultraviolet photodiode array detection for analysis of flavonoid glycosides. *Rapid Commun. Mass Spectrom.*, **16(24)**, 2341-2348 (2002).
8. Slys, G. W., and Schriemer, D. C., On-column digestion of proteins in aqueous-organic solvents. *Rapid Commun. Mass Spectrom.*, **17(10)**, 1044-1050 (2003).
9. Marcotte, F. A., et al., Diversity-oriented synthesis of functionalized pyrrolo[3,2-*d*]pyrimidines with variation of the pyrimidine ring nitrogen substituents. *J. Org. Chem.*, **68(18)**, 6984-6987 (2003).
10. Bratt, M. O., and Taylor, P. C., Synthesis of carbonates and related compounds from carbon dioxide via methanesulfonyl carbonates. *J. Org. Chem.*, **68(14)**, 5439-5444 (2003).
11. Fillon, H., et al., New chemical synthesis of functionalized arylzinc compounds from aromatic or thienyl bromides under mild conditions using a simple cobalt catalyst and zinc dust. *J. Am. Chem. Soc.*, **125(13)**, 3867-3870 (2003).
12. Nather, C., and Jess, I., Synthesis, crystal structures, and thermal and thermodynamic properties of dimorphic copper(I) coordination polymers. *Inorg. Chem.*, **42(9)**, 2968-2976 (2003).
13. Bennett, B. K., et al., Osmium phosphinimato complexes: synthesis, protonation, structure, and redox-coupled hydrolytic scission of N-p bonds. *Inorg. Chem.*, **42(13)**, 4127-4134 (2003).
14. Zuo, J. L., et al., Vanadium-iron-sulfur clusters containing the cubane-type [VFe₃S₄] core unit: synthesis of a cluster with the topology of the PN cluster of nitrogenase. *Inorg. Chem.*, **42(15)**, 4624-4631 (2003).

GCY/RXR 11/03

Sigma brand products are sold through Sigma-Aldrich, Inc.

Sigma-Aldrich, Inc. warrants that its products conform to the information contained in this and other Sigma-Aldrich publications. Purchaser must determine the suitability of the product(s) for their particular use. Additional terms and conditions may apply. Please see reverse side of the invoice or packing slip.