Specification Sheet

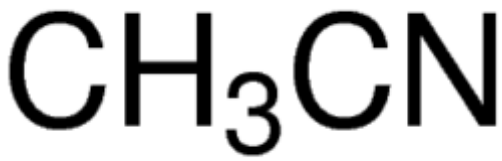
34998 Sigma-Aldrich

Acetonitrile

HPLC Plus, ≥99.9%

Synonym: **ACN, Cyanomethane, Ethyl nitrile, Methyl cyanide**

- **CAS Number** 75-05-8
- **Linear Formula** CH_3CN
- **Molecular Weight** 41.05
- **Beilstein/REAXYS Number** 741857
- **EC Number** 200-835-2
- **MDL number** MFCD00001878
- **eCl@ss** 39031501
- **PubChem Substance ID** 329755104
- **NACRES** NA.03



SKU-Pack Size	Availability	Pack Size	Price (SGD)	Quantity
34998-1L	Estimated to ship on 28.04.2021 - FROM	1 L	199.24	0
34998-2.5L	Estimated to ship on 05.05.2021 - FROM	2.5 L	297.56	0
34998-6X1L	Estimated to ship on 04.05.2021 - FROM	6 x 1 L	905.62	0
34998-4X2.5L	Estimated to ship on 04.05.2021 - FROM	4 x 2.5 L	991.87	0

Properties

Related Categories Acetonitrile and Acetonitrile Solutions, Analytical Reagents, Analytical/Chromatography, Chromatography Reagents, HPLC Plus Grade Solvents,

Quality Level	100
grade	**HPLC Plus**
vapor density	**1.41 (vs air)**
vapor pressure	**72.8 mmHg (20 °C)**
assay	**≥99.9%**
form	**liquid**
autoignition temp.	**973 °F**
expl. lim.	**16 %**
baseline drift measuring range	**≤12 mAU (210 nm)**
application(s)	**HPLC: suitable**
	IR spectroscopy: suitable
impurities	**≤0.0001% free alkali (as NH_3)**
	≤0.0002% non-volatile matter
	≤0.001% free acid (as CH_3COOH)
	≤0.01% water (Karl Fischer)
	≤0.5 ppb fluorescence (quinine) at 254 nm
	≤0.5 ppb fluorescence (quinine) at 365 nm
halogenated residue	**10 ng/L (as heptachlor epoxide)**
refractive index	***n*20/D 1.344 (lit.)**

bp	**81-82 °C (lit.)**
mp	**−45 °C (lit.)**
density	**0.786 g/mL at 25 °C (lit.)**
HPLC-gradient	**≤0.2 mAU at 254 nm**
	≤1 mAU at 210 nm
λ	**H_2O reference**
UV absorption	**λ: 195 nm A_{max}: ≤0.10**
	λ: 200 nm A_{max}: ≤0.02
	λ: 228 nm A_{max}: ≤0.005
	λ: 235 nm A_{max}: ≤0.0044
	λ: 250 nm A_{max}: ≤0.0044
	λ: 400 nm A_{max}: ≤0.0044
Featured Industry	**Food and Beverages**
storage temp.	**room temp**
SMILES string	**CC#N**
InChI	**1S/C2H3N/c1-2-3/h1H3**
InChI key	**WEVYAHXRMPXWCK-UHFFFAOYSA-N**

Show Fewer Properties

Description

General description

Acetonitrile (MeCN) is widely employed as a solvent in various studies and has high dielectric constant (37.5). Various purification procedures to obtain different grades of acetonitrile for use in different studies (polarography, spectroscopy, etc.) have been reported by many researchers.[2]

Application

Acetonitrile has been used to compose the gradient system for the HPLC detection of diphenylmethane diisocyanate, a polymeric degradation product.[1]

New Quality UPLC Plus Acetonitrile is suitable for all applications including:

Mass spectrometry, HPLC, TLC, GPC, UV, IR, GC, Pesticide Residue Analysis, and RNA/DNA Synthesis and Purification.

Packaging

1, 6×1, 2.5, 4×2.5, 4, 4×4 L in glass bottle

20 L in Nowpak™

20, 50 L in Pure-Pac™ 2

200 L in Pure-Pac™ 1

View returnable container options.

200 L in Pure-Pac™ 2

Preparation Note

Product filtered through a 0.2 µm filter

Other Notes

Pure-Pac® II containers require the Micromatic MacroValve coupler for dispensing solvents, Z560723.

Important notice

• The article number 34998-4X2.5L will be discontinued. Please order the single bottle 34998-2.5L which is physically identical with the same exact specifications.

• The article number 34998-6X1L will be discontinued. Please order the single bottle 34998-1L which is physically identical with the same exact specifications.

Recommended products

Discover LiChropur reagents ideal for **HPLC** or **LC-MS** analysis

Legal Information

Pure-Pac is a registered trademark of Sigma-Aldrich Co. LLC