

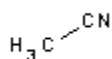


PRODUCT CODE: 221881

Acetonitrile (Reag. USP, Ph. Eur.) for HPLC gradient / UHPLC supergradient grade, ACS

C₂H₃N

CH₃CN



M.= 41,05

CAS [75-05-8]

EINECS 200-835-2

TARIC 2926 90 70 90

SYNONYMS: Cyanomethane, Ethanenitrile, Methyl Cyanide

PHYSICAL DATA: liquid, Clear, Colourless, Miscible with water • Hygroscopic • D 20/4 0,786 • M.P.: -48 °C • B.P.: 80 - 82 °C • n_{20/D} : 1,344 • Flash P.:12,8 °C(closed cup) • Ign. T.:524 °C • Vap. press. (20 °C) 98,64 hPa (25 °C) 121,44 hPa • Viscosity 20 °C 0,35 mPa.s • D. M. 20 °C 3,44 Debye • Dielec. constant 20 °C 38,8 • Heat evap. 82 °C 833 KJ/Kg • Satur. conc. 20 °C 163 g/m³ • Expl. limit 3 % (V) 16 % (V) •

BIBLIOGRAPHY: Merck Index **13**, 71 Sax **ABE500** • Safety **2**, **22 A** • Kühn-Birett **A 5** • Beilstein **2**, **183 I**, **184 II**, **181 III**, **408 IV**, **419** • BRN 741857 • Fieser **213** • ACS **XI** •

HAZARDOUS: C.E: 608-001-00-3 • RTECS: AL 7700000 • LD50 oral mus 617 mg/kg / (OECD 401) • LC50 mus 6,022 mg/l / 4h, (OECD 403) • LD50 skn rbt >2.000 mg/kg / (OECD 402) • ECTLV 40 ppm 70 mg/m³ VLA-ED 40 ppm 68 mg/m³ Factor for short-term value (Germany) 2

Derived No Effect Level (DNEL)

Workers Inhalation, acute (systemic) 68 mg/m³ Workers Inhalation, acute (local) 68 mg/m³ Workers Dermal, long exposure (systemic) 32.2mg/kg Workers Inhalation, long term (systemic) 68 mg/m³ Workers Inhalation, long term (local) 68 mg/m³ Population Inhalation, acute (systemic) 220 mg/m³ Population, oral, acute (systemic) 0.6mg/kg Population Inhalation, acute (local) 22 mg/m³ Population Inhalation, long term (systemic) 4,8 mg/m³ Population Inhalation, long term (local) 4,8 mg/m³

Predicted No Effect Concentration (PNEC)

Freshwater 10mg/l Marine water 1mg/l Periodic release 10mg/l Freshwater Sediment 7.53mg/kg Soil 2.41mg/kg Sewage treatment plant 32mg/l



H: H225 • H332 • H312 • H302 • H319 •

P: P210 • P233 • P240 • P241 • P242 • P243 • P261 • P270 • P271 • P280 • P301+P330+P331 • P303+P361+P353 • P304+P340 • P305+P351+P338 • P337+P313 • P312 • P322 • P363 • P370+P378 • P501 •

TRANSPORT REGULATIONS: UN: 1648 • ADR: 3/II • IMDG: 3/II • IATA: 3/II • PAX: 353 • CAO: 364 • (D/E) •

WEIGHT/VOLUME INFORMATION: 1l-0,781 kg 1kg-1,28 l

SPECIFICATIONS:

Minimum assay (G.C.)	99,9%
Identity :	
Identity	IR passes test
Density at 20/4	0,779-0,783
Suitability: for gradient acc. to ACS	passes test
Range of Distillation (>95% dist.)	80-82°C

Maximum limit of impurities

APHA colour	10
Acidity	0,0005 meq/g
Alkalinity	0,0001 meq/g
Non-volatile matter	0,0001 %
Base line drift (210 nm)	10 mUA
Water (H ₂ O)	0,015 %
Gradient at 210 nm	1 mUA
Gradient at 254 nm	0,5 mUA
Fluorescence at 254 nm (as quinine)	1 ppb
Fluorescence at 365 nm (as quinine)	0,5 ppb
UV Spectrum (1cm cell; Ref.: water):	
Transmittance at 190 (Cut off) nm	≥ 30 %
Transmittance at 193 nm	≥ 60 %
Transmittance at 195 nm	≥ 80 %
Transmittance at 200 nm	≥ 90 %
Transmittance at 230-400 nm	≥ 98 %

Data of interest in HPLC:	
Rohrschneider Polarity	5,8
Eluotropic value E° (Al ₂ O ₃)	0,65
Sol. H ₂ O in solv. at 20°C	miscible

Microfiltered product (0.2 µm) and bottled under nitrogen atmosphere.

Conforms to Acetonitrile for chromatography and Acetonitrile R1 according to Reag. Ph. Eur.