

Safety Data Sheet

according to Regulation (EC) No 1907/2006

4,4-Nitrobenzylpyridin 5 % (m/V) zur Synthese in Aceton

Revision date: 07.09.2023

Product code: 33826

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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

4,4-Nitrobenzylpyridin 5 % (m/V) zur Synthese in Aceton

UFI: 04P0-R3A5-S00X-AKTH

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the substance/mixture

Laboratory chemical

Industrial uses: Uses of substances as such or in preparations at industrial sites

Professional uses: Public domain (administration, education, entertainment, services, craftsmen)

Uses advised against

Do not use for private purposes (household).

1.3. Details of the supplier of the safety data sheet

Company name:	AnalytiChem GmbH	
Street:	Stempelstraße 6	
Place:	D-47167 Duisburg	
Telephone:	0203/5194-0	Telefax: 0203/5194-290
E-mail:	info@analytichem.de	
Contact person:	Abteilung Produktsicherheit	Telephone: 0203/5194-107/117
E-mail:	produktsicherheit@analytichem.de	
Internet:	www.analytichem.de	
Responsible Department:	Abteilung Produktsicherheit	

1.4. Emergency telephone number:

For Hazardous Materials [or Dangerous Goods] Incidents Spill, Leak, Fire, Exposure, or Accident Call CHEMTREC Day or Night Within USA and Canada: 1-800-424-9300 Outside USA and Canada: +1 703-741-5970 (collect calls accepted)

Further Information

This product is a mixture. REACH Registration Number see section 3.

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Regulation (EC) No 1272/2008

Flam. Liq. 2; H225

Eye Irrit. 2; H319

STOT SE 3; H336

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Hazard components for labelling

acetone

Signal word: Danger

Pictograms:



Hazard statements

H225

Highly flammable liquid and vapour.

H319

Causes serious eye irritation.

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H336 May cause drowsiness or dizziness.

Precautionary statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
 P233 Keep container tightly closed.
 P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
 P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
 P337+P313 If eye irritation persists: Get medical advice/attention.
 P403+P235 Store in a well-ventilated place. Keep cool.

Special labelling of certain mixtures

EUH066 Repeated exposure may cause skin dryness or cracking.

2.3. Other hazards

No information available.

SECTION 3: Composition/information on ingredients

3.2. Mixtures

Hazardous components

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
67-64-1	acetone			90 - < 95 %
	200-662-2	606-001-00-8	01-2119471330-49	
	Flam. Liq. 2, Eye Irrit. 2, STOT SE 3; H225 H319 H336 EUH066			

Full text of H and EUH statements: see section 16.

Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
	Specific Conc. Limits, M-factors and ATE		
67-64-1	200-662-2	acetone	90 - < 95 %
	dermal: LD50 = > 7426 mg/kg; oral: LD50 = 5800 mg/kg		

Further Information

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of = 0.1 % (w/w).

SECTION 4: First aid measures

4.1. Description of first aid measures

General information

No data available

After inhalation

Provide fresh air.
 Call a physician immediately.

After contact with skin

Wash immediately with: Water
 Take off immediately all contaminated clothing and wash it before reuse.

After contact with eyes

After contact with the eyes, rinse with water with the eyelids open for a sufficient length of time, then consult an ophthalmologist immediately.

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Remove contact lenses, if present and easy to do. Continue rinsing.

After ingestion

Observe risk of aspiration if vomiting occurs.
Call a physician immediately.

4.2. Most important symptoms and effects, both acute and delayed

Irritant, Dizziness, Anaesthetic state
Vomiting, Headache, Dizziness
Gastrointestinal complaints, Corneal opacity.
Has degreasing effect on the skin.
Repeated exposure may cause skin dryness or cracking.
May cause drowsiness or dizziness.

4.3. Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂).
Foam.
Extinguishing powder

Unsuitable extinguishing media

no restriction

5.2. Special hazards arising from the substance or mixture

Combustible liquid.
Vapours are heavier than air, spread along floors and form explosive mixtures with air.
Hazardous combustion products
In case of fire may be liberated: Carbon dioxide (CO₂), Carbon monoxide
Beware of reignition.

5.3. Advice for firefighters

Remove persons to safety. Do not inhale explosion and combustion gases.
Avoid contact with skin, eyes and clothes.
In case of fire: Wear self-contained breathing apparatus.
Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.

Additional information

Danger of bursting container.
Use water spray jet to protect personnel and to cool endangered containers.
Suppress gases/vapours/mists with water spray jet.
Move undamaged containers from immediate hazard area if it can be done safely.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General advice

Keep away from sources of ignition - No smoking.
This material can be ignited by heat, sparks, flames, or other sources of ignition (e.g., static electricity, pilot lights, mechanical/electrical equipment, and electronic devices such as cell phones, computers, calculators, and pagers which have not been certified as intrinsically safe).
Take action to prevent static discharges.

For non-emergency personnel

Provide adequate ventilation.
Use personal protection equipment.
Avoid contact with skin, eyes and clothes.

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Remove persons to safety.
Emergency procedures
Do not breathe dust/fume/gas/mist/vapours/spray.

For emergency responders

Precautionary statements For emergency responders : Personal protection equipment: see section 8

6.2. Environmental precautions

Do not allow to enter into surface water or drains.
The vapour of the product is heavier than air and may accumulate below ground level, in pits, channels and basements in higher concentration.
Danger of explosion

6.3. Methods and material for containment and cleaning up

For containment

Cover drains.
Prevent spread over a wide area (e.g. by containment or oil barriers).
Collect in closed and suitable containers for disposal.
Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

For cleaning up

Clean contaminated articles and floor according to the environmental legislation.

Other information

Provide adequate ventilation.
Do not breathe dust/fume/gas/mist/vapours/spray.
Wear breathing apparatus if exposed to vapours/dusts/aerosols.

6.4. Reference to other sections

Safe handling: see section 7
Personal protection equipment: see section 8
Disposal: see section 13

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

If handled uncovered, arrangements with local exhaust ventilation have to be used.
Read label before use. Handle and open container with care.
When using do not eat, drink, smoke, sniff. Keep container tightly closed.
Use personal protection equipment. Use extractor hood (laboratory).
Do not breathe vapour/aerosol. Provide adequate ventilation.

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking.
Take precautionary measures against static discharges.
Vapours can form explosive mixtures with air.

Advice on general occupational hygiene

Draw up and observe skin protection programme. Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat or drink.
Keep away from food, drink and animal feedingstuffs.
Take off immediately all contaminated clothing.
Wash hands before breaks and after work.

Further information on handling

Take off immediately all contaminated clothing and wash it before reuse.
Draw up and observe skin protection programme.
Wash hands and face before breaks and after work and take a shower if necessary.

7.2. Conditions for safe storage, including any incompatibilities

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Requirements for storage rooms and vessels

Keep container tightly closed. Keep in a cool, well-ventilated place. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
storage temperature: +5°C - +30°C

Further information on storage conditions

Keep cool. Protect from sunlight.
Protect against: Light

7.3. Specific end use(s)

Laboratory chemicals

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Occupational exposure limits

CAS No	Substance	ppm	mg/m ³	fib/cm ³	Category	Origin
67-64-1	Acetone	500	1210		TWA (8 h)	

Biological limit values

CAS No	Substance	Parameter	Value	Test material	Sampling time
67-64-1	Acetone	Acetone	50 mg/L	Urine	End of shift

DNEL/DMEL values

CAS No	Substance	DNEL type	Exposure route	Effect	Value
67-64-1	acetone	Worker DNEL, long-term	inhalation	systemic	1210 mg/m ³
		Worker DNEL, acute	inhalation	local	2420 mg/m ³
		Worker DNEL, long-term	dermal	systemic	186 mg/kg bw/day
		Consumer DNEL, long-term	inhalation	systemic	200 mg/m ³
		Consumer DNEL, long-term	dermal	systemic	62 mg/kg bw/day
		Consumer DNEL, long-term	oral	systemic	62 mg/kg bw/day

PNEC values

CAS No	Substance	Environmental compartment	Value
67-64-1	acetone	Freshwater	10,6 mg/l
		Freshwater (intermittent releases)	21 mg/l
		Marine water	1,06 mg/l
		Freshwater sediment	30,4 mg/kg
		Marine sediment	3,04 mg/kg
		Micro-organisms in sewage treatment plants (STP)	100 mg/l
		Soil	29,5 mg/kg

8.2. Exposure controls

Appropriate engineering controls

Technical measures and the application of suitable work processes have priority over personal protection

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equipment.

If handled uncovered, arrangements with local exhaust ventilation have to be used.

Do not breathe vapour/aerosol.

Individual protection measures, such as personal protective equipment

Eye/face protection

Suitable eye protection: goggles.

Face protection umbrella

Hand protection

Protective gloves are recommended Company KCL GmbH, D-36124 Eichenzell, email: vertrieb@kcl.de With specification (test according to EN374):

By long-term hand contact

Trade name/designation: KCL 897 Butoject®

Suitable material: Butyl caoutchouc (butyl rubber) 0,3 mm

Wearing time with permanent contact: > 480 min

By short-term hand contact

Trade name/designation: KCL 897 Butoject®

Suitable material: Butyl caoutchouc (butyl rubber) 0,3 mm

Wearing time with occasional contact (splashes): > 480 min

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types. This recommendation applies only to the product stated in the safety data sheet supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Skin protection

Flame-retardant protective clothing. Wear anti-static footwear and clothing

Take off immediately all contaminated clothing.

Wash hands before breaks and after work.

Draw up and observe skin protection programme.

Respiratory protection

Respiratory protection necessary at: aerosol or mist formation

Environmental exposure controls

Do not allow to enter into surface water or drains.

Due to danger of explosion, prevent leakage of vapours into cellars, flues and ditches.

Danger of explosion

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state:	Liquid
Colour:	yellow
Odour:	fruity
Odour threshold:	No data available
Melting point/freezing point:	-95,4 °C
Boiling point or initial boiling point and boiling range:	56,2 °C
Flammability:	not applicable
Lower explosion limits:	2,15 vol. %
Upper explosion limits:	13 vol. %

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Flash point:	<-20 °C
Auto-ignition temperature:	465 °C
Decomposition temperature:	No data available
pH-Value (at 20 °C):	6,4
Viscosity / kinematic:	No data available
Water solubility:	No data available
Solubility in other solvents	
No data available	
Dissolution rate:	No data available
Partition coefficient n-octanol/water:	No data available
Dispersion stability:	No data available
Vapour pressure:	No data available
Vapour pressure:	No data available
Density (at 20 °C):	0,81 g/cm ³
Relative density:	No data available
Bulk density:	No data available
Relative vapour density:	No data available
Particle characteristics:	No data available

9.2. Other information

Information with regard to physical hazard classes

Explosive properties

Vapours can form explosive mixtures with air.

Sustaining combustion:

Sustaining combustion

Self-ignition temperature

Solid:

not applicable

Gas:

not applicable

Oxidizing properties

No data available

Other safety characteristics

Evaporation rate:

No data available

Solvent separation test:

No data available

Solvent content:

No data available

Solid content:

No data available

Sublimation point:

No data available

Softening point:

No data available

Pour point:

No data available

No data available:

Viscosity / dynamic:

No data available

Flow time:

No data available

Further Information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

Highly flammable.

Vapours can form explosive mixtures with air.

10.2. Chemical stability

Protect against:

Light

Air

10.3. Possibility of hazardous reactions

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Ignition hazard:
Fluorine, Oxidising agent, strong;
Reducing agent, strong; Nitric acid
Danger of explosion:
Chloroform, peroxides, for example hydrogen peroxide
Exothermic reaction with:
Bromine, Alkali metals
Hydrogen halide, Sulphur dichloride

10.4. Conditions to avoid

Heat
Light
Air

10.5. Incompatible materials

Rubber articles
Plastic articles

10.6. Hazardous decomposition products

SECTION 5: Firefighting measures

Further information

No data available

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Toxicokinetics, metabolism and distribution

There are no data available on the mixture itself.

Acute toxicity

Based on available data, the classification criteria are not met.

ATEmix calculated

ATE (oral) > 2000 mg/kg; ATE (dermal) > 2000 mg/kg; ATE (inhalation vapour) > 20 mg/l; ATE (inhalation dust/mist) > 5 mg/l

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
67-64-1	acetone				
	oral	LD50 5800 mg/kg	Rat	J Toxicol Environ Health 15: 609-621 (19)	Undiluted acetone applied to female rats
	dermal	LD50 > 7426 mg/kg	Rabbit	Toxicol Appl Pharmacol 7: 559-565. (1965)	other: Code of federal regulations: 21 C

Irritation and corrosivity

Causes serious eye irritation.
Skin corrosion/irritation: Based on available data, the classification criteria are not met.
Has degreasing effect on the skin.
Repeated exposure may cause skin dryness or cracking.

Sensitising effects

Based on available data, the classification criteria are not met.

Carcinogenic/mutagenic/toxic effects for reproduction

Based on available data, the classification criteria are not met.

STOT-single exposure

May cause drowsiness or dizziness. (acetone)

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STOT-repeated exposure

Repeated exposure may cause skin dryness or cracking.

Aspiration hazard

Based on available data, the classification criteria are not met.

Information on likely routes of exposure

There are no data available on the mixture itself.

Specific effects in experiment on an animal

There are no data available on the mixture itself.

Additional information on tests

There are no data available on the mixture itself.

Practical experience

There are no data available on the mixture itself.

11.2. Information on other hazards

Endocrine disrupting properties

There are no data available on the mixture itself.

Other information

There are no data available on the mixture itself.

Further information

Irritant, Dizziness, Anaesthetic state
Vomiting, Headache, Dizziness
Gastrointestinal complaints, Corneal opacity.
Has degreasing effect on the skin.
Repeated exposure may cause skin dryness or cracking.
May cause drowsiness or dizziness.

SECTION 12: Ecological information

12.1. Toxicity

There are no data available on the mixture itself.

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
67-64-1	acetone					
	Acute fish toxicity	LC50 8120 mg/l	96 h	Pimephales promelas	Publication (1984)	OECD Guideline 203
	Acute crustacea toxicity	EC50 8800 mg/l	48 h	Daphnia pulex	Publication (1978)	The toxicity of acetone towards daphnids
	Crustacea toxicity	NOEC 2212 mg/l	28 d	Daphnia magna	Arch Environm Contam Toxicol 12: 305-310	Study conducted comparable to OECD 211 w
	Acute bacteria toxicity	(EC50 61150 mg/l)	0,5 h	activated sludge of a predominantly domestic sewage	Water Res 26: 887-892 (1992)	ISO 8192

12.2. Persistence and degradability

There are no data available on the mixture itself.

12.3. Bioaccumulative potential

There are no data available on the mixture itself.

Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
67-64-1	acetone	-0,23

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BCF

CAS No	Chemical name	BCF	Species	Source
67-64-1	acetone	3		Unpublished calculat

12.4. Mobility in soil

There are no data available on the mixture itself.

12.5. Results of PBT and vPvB assessment

The substances in the mixture do not meet the PBT/vPvB criteria according to REACH, annex XIII.

12.6. Endocrine disrupting properties

This product does not contain a substance that has endocrine disrupting properties with respect to non-target organisms as no components meets the criteria.

12.7. Other adverse effects

Avoid release to the environment.

Further information

Do not allow to enter into surface water or drains.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal recommendations

Waste disposal according to directive 2008/98/EC, covering waste and dangerous waste.
Send to a physico-chemical treatment facility under observation of official regulations.
Do not empty into drains.

Contaminated packaging

Handle contaminated packages in the same way as the substance itself.
The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

SECTION 14: Transport information

Land transport (ADR/RID)

14.1. UN number or ID number:	UN 1090
14.2. UN proper shipping name:	ACETONE
14.3. Transport hazard class(es):	3
14.4. Packing group:	II
Hazard label:	3
Classification code:	F1
Limited quantity:	1 L
Excepted quantity:	E2
Transport category:	2
Hazard No:	33
Tunnel restriction code:	D/E

Inland waterways transport (ADN)

14.1. UN number or ID number:	UN 1090
14.2. UN proper shipping name:	ACETONE
14.3. Transport hazard class(es):	3
14.4. Packing group:	II
Hazard label:	3
Classification code:	F1
Limited quantity:	1 L
Excepted quantity:	E2

Marine transport (IMDG)

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14.1. UN number or ID number:	UN 1090
14.2. UN proper shipping name:	ACETONE
14.3. Transport hazard class(es):	3
14.4. Packing group:	II
Hazard label:	3
Special Provisions:	-
Limited quantity:	1 L
Excepted quantity:	E2
EmS:	F-E, S-D

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number:	UN 1090
14.2. UN proper shipping name:	ACETONE
14.3. Transport hazard class(es):	3
14.4. Packing group:	II
Hazard label:	3
Limited quantity Passenger:	1 L
Passenger LQ:	Y341
Excepted quantity:	E2
IATA-packing instructions - Passenger:	353
IATA-max. quantity - Passenger:	5 L
IATA-packing instructions - Cargo:	364
IATA-max. quantity - Cargo:	60 L

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

14.6. Special precautions for user

Warning: Combustible liquid.

14.7. Maritime transport in bulk according to IMO instruments

not applicable

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

EU regulatory information

Restrictions on use (REACH, annex XVII):

Entry 3, Entry 40

Information according to 2012/18/EU (SEVESO III): P5c FLAMMABLE LIQUIDS

Marketing and use of explosives precursors (Regulation (EU) 2019/1148):

This product is regulated by Regulation (EU) 2019/1148: all suspicious transactions, and significant disappearances and thefts should be reported to the relevant national contact point.

Additional information

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of = 0.1 % (w/w).

National regulatory information

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC).

Water hazard class (D): 1 - slightly hazardous to water

SECTION 16: Other information

Changes

This data sheet contains changes from the previous version in section(s): 1,2,3,8,9,11,12.

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Abbreviations and acronyms

ADR: Accord européen sur le transport des marchandises dangereuses par Route
(European Agreement concerning the International Carriage of Dangerous Goods by Road)
IMDG: International Maritime Code for Dangerous Goods
IATA: International Air Transport Association
GHS: Globally Harmonized System of Classification and Labelling of Chemicals
EINECS: European Inventory of Existing Commercial Chemical Substances
ELINCS: European List of Notified Chemical Substances
CAS: Chemical Abstracts Service
LC50: Lethal concentration, 50%
LD50: Lethal dose, 50%
Flam. Liq: Flammable liquid
Eye Irrit: Eye irritation
STOT SE: Specific target organ toxicity - single exposure

Classification for mixtures and used evaluation method according to Regulation (EC) No 1272/2008 [CLP]

Classification	Classification procedure
Flam. Liq. 2; H225	On basis of test data
Eye Irrit. 2; H319	Calculation method
STOT SE 3; H336	Calculation method

Relevant H and EUH statements (number and full text)

H225 Highly flammable liquid and vapour.
H319 Causes serious eye irritation.
H336 May cause drowsiness or dizziness.
EUH066 Repeated exposure may cause skin dryness or cracking.

(The data for the hazardous ingredients were taken respectively from the last version of the sub-contractor's safety data sheet.)