

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifier**

Trade name **Hexanes, mixed isomers, ACS**  
 Stock number: 33321  
 CAS Number: 92112-69-1

**1.2 Relevant identified uses of the substance**

or mixture and uses advised against. No further relevant information available.  
 Identified use: SU24 Scientific research and development

**1.3 Details of the supplier of the safety data sheet**

Manufacturer/Supplier: Alfa Aesar GmbH & Co.KG  
 A Johnson Matthey Company  
 Zeppelinstr. 7b  
 76185 Karlsruhe / Germany  
 Tel: +49 (0) 721 84007 280  
 Fax: +49 (0) 721 84007 300  
 Email: tech@alfa.com  
 www.alfa.com  
 Product safety Tel + +049 (0) 7275 988687-0  
 Carechem 24: +44 (0) 1235 239 670 (Multi-language emergency number)  
 Poison Information Center Mainz  
 www.giftinfo.uni-mainz.de Telephone: +49(0)6131/19240


Informing department:

**1.4 Emergency telephone number:****SECTION 2: Hazards identification****2.1 Classification of the substance or mixture**

Classification according to Regulation (EC) No 1272/2008

 GHS02 flame


Flam. Liq. 2 H225 Highly flammable liquid and vapour.

 GHS08 health hazard

Repr. 2 H361f Suspected of damaging fertility.

STOT RE 2 H373 May cause damage to the peripheral nervous system, the lung, the kidneys, the liver, the reproductive system and the brain through prolonged or repeated exposure. Route of exposure: Inhalative.

Asp. Tox. 1 H304 May be fatal if swallowed and enters airways.

 GHS09 environment


Aquatic Chronic 2 H411 Toxic to aquatic life with long lasting effects.

 GHS07


Skin Irrit. 2 H315 Causes skin irritation.

STOT SE 3 H336 May cause drowsiness or dizziness.


**Classification according to Directive 67/548/EEC or Directive 1999/45/EC**

 Xn; Harmful


R48/20-62-65: Harmful: danger of serious damage to health by prolonged exposure through inhalation. Possible risk of impaired fertility. Harmful: may cause lung damage if swallowed.

 Xi; Irritant

R38: Irritating to skin.

 F; Highly flammable

R11: Highly flammable.

 N; Dangerous for the environment

R51/53: Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

R67: Vapours may cause drowsiness and dizziness.

**Information concerning particular hazards for human and environment:**

The product has to be labelled due to the calculation procedure of the "General Classification guideline for preparations of the EU" in the latest valid version.  
 Has a narcotizing effect.

**Other hazards that do not result in classification**

No information known.

**2.2 Label elements****Labelling according to Regulation (EC) No 1272/2008****Hazard pictograms****Signal word****Hazard-determining components of labelling:****Hazard statements**

The product is classified and labelled according to the CLP regulation.

GHS02, GHS07, GHS08, GHS09

Danger

n-Hexane

3-Methylpentane

H225 Highly flammable liquid and vapour.

H315 Causes skin irritation.

H361f Suspected of damaging fertility.

H336 May cause drowsiness or dizziness.

H373 May cause damage to the peripheral nervous system, the lung, the kidneys, the liver, the reproductive system and the brain through prolonged or repeated exposure. Route of exposure: Inhalative.

H304 May be fatal if swallowed and enters airways.

H411 Toxic to aquatic life with long lasting effects.

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

P241 Use explosion-proof electrical/ventilating/lighting/equipment.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower.

P405 Store locked up.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

**Precautionary statements****2.3 Other hazards****Results of PBT and vPvB assessment**

PBT: Not applicable.

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vPvB: Not applicable.

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**SECTION 3: Composition/information on ingredients****3.2 Mixtures****Dangerous components:**

CAS: 110-54-3 EINECS: 203-777-6	n-Hexane Xn R48/20-62-65; Xi R38; F R11; N R51/53 R67 Repr. Cat. 3 Flam. Liq. 2, H225; Repr. 2, H361f; STOT RE 2, H373; Asp. Tox. 1, H304; Aquatic Chronic 2, H411; Skin Irrit. 2, H315; STOT SE 3, H336	65,0%
CAS: 96-14-0 EINECS: 202-481-4	3-Methylpentane Xn R65; Xi R38; F R11; N R51/53 R67 Flam. Liq. 2, H225; Asp. Tox. 1, H304; Aquatic Chronic 2, H411; Skin Irrit. 2, H315; STOT SE 3, H336	25,0%
CAS: 107-83-5 EINECS: 203-523-4	2-Methylpentane Xn R65; Xi R38; F R11; N R51/53 R67 Flam. Liq. 2, H225; Asp. Tox. 1, H304; Aquatic Chronic 2, H411; Skin Irrit. 2, H315; STOT SE 3, H336	5,0%
CAS: 96-37-7 EINECS: 202-503-2	Methylcyclopentane Xi R36/37/38; F R11 Flam. Liq. 2, H225; Skin Irrit. 2, H315; Eye Irrit. 2, H319; STOT SE 3, H335	4,999%

**Additional information** None known.**Non-Hazardous Ingredients**

CAS: 71-43-2 EINECS: 200-753-7	Benzene T Carc. Cat. 1, Muta. Cat. 2 R45-46-48/23/24/25; Xn R65; Xi R36/38; F R11 Flam. Liq. 2, H225; Muta. 1B, H340; Carc. 1A, H350; STOT RE 1, H372; Asp. Tox. 1, H304; Skin Irrit. 2, H315; Eye Irrit. 2, H319	0,001%
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**SECTION 4: First aid measures****4.1 Description of first aid measures****After inhalation**

Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.

**After skin contact**Seek immediate medical advice.  
Instantly wash with water and soap and rinse thoroughly.**After eye contact**

Seek immediate medical advice.

**After swallowing**

Rinse opened eye for several minutes under running water. Then consult doctor.

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

No further relevant information available.

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

No further relevant information available.

**SECTION 5: Firefighting measures****5.1 Extinguishing media****Suitable extinguishing agents**

Use carbon dioxide, extinguishing powder or foam. Water may be ineffective but may be used for cooling exposed containers.

**5.2 Special hazards arising from the substance or mixture**If this product is involved in a fire, the following can be released:  
Carbon monoxide and carbon dioxide**5.3 Advice for firefighters  
Protective equipment:**Wear self-contained breathing apparatus.  
Wear full protective suit.**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**Wear protective equipment. Keep unprotected persons away.  
Ensure adequate ventilation**6.2 Environmental precautions:**Keep away from ignition sources  
Do not allow material to be released to the environment without proper governmental permits.  
Do not allow product to reach sewage system or water bodies.  
Do not allow to enter the ground/soil.**6.3 Methods and material for containment and cleaning up:**Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).  
Dispose of contaminated material as waste according to item 13.  
Ensure adequate ventilation.**Prevention of secondary hazards:**

Keep away from ignition sources.

**6.4 Reference to other sections**See Section 7 for information on safe handling  
See section 8 for information on personal protection equipment.  
See Section 13 for information on disposal.**SECTION 7: Handling and storage****7.1 Precautions for safe handling**Keep containers tightly sealed.  
Store in cool, dry place in tightly closed containers.  
Ensure good ventilation/exhaustion at the workplace.**Information about protection against explosions and fires:**Protect against electrostatic charges.  
Fumes can combine with air to form an explosive mixture.**7.2 Conditions for safe storage, including any incompatibilities****Storage  
Requirements to be met by storerooms and containers:**

Store in cool location.

**Information about storage in one common storage facility:**

Store away from oxidizing agents.

**Further information about storage conditions:**Keep container tightly sealed.  
Store in cool, dry conditions in well sealed containers.**7.3 Specific end use(s)**

No further relevant information available.

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**SECTION 8: Exposure controls/personal protection****Additional information about design of technical systems:**

Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

**8.1 Control parameters****Components with critical values that require monitoring at the workplace:****110-54-3 n-Hexane (65,0%)**

AGW (Germany)	180 mg/m <sup>3</sup> , 50 ppm 8(II);DFG, EU, Y
PEL (USA)	1800 mg/m <sup>3</sup> , 500 ppm
REL (USA)	180 mg/m <sup>3</sup> , 50 ppm
TLV (USA)	176 mg/m <sup>3</sup> , 50 ppm Skin; BEI

**96-14-0 3-Methylpentane (25,0%)**

AGW (Germany)	1800 mg/m <sup>3</sup> , 500 ppm 2(II);DFG
REL (USA)	Short-term value: C 1800* mg/m <sup>3</sup> , C 510* ppm Long-term value: 350 mg/m <sup>3</sup> , 100 ppm *15-min
TLV (USA)	Short-term value: 3500 mg/m <sup>3</sup> , 1000 ppm Long-term value: 1760 mg/m <sup>3</sup> , 500 ppm

**107-83-5 2-Methylpentane (5,0%)**

AGW (Germany)	1800 mg/m <sup>3</sup> , 500 ppm 2(II);DFG
REL (USA)	Short-term value: C 1800* mg/m <sup>3</sup> , C 510* ppm Long-term value: 350 mg/m <sup>3</sup> , 100 ppm *15-min
TLV (USA)	Short-term value: 3500 mg/m <sup>3</sup> , 1000 ppm Long-term value: 1760 mg/m <sup>3</sup> , 500 ppm

**96-37-7 Methylcyclopentane (4,999%)**

AGW (Germany)	1800 mg/m <sup>3</sup> , 500 ppm 2(II);DFG
REL (USA)	Short-term value: C 1800* mg/m <sup>3</sup> , C 510* ppm Long-term value: 350 mg/m <sup>3</sup> , 100 ppm *15-min
TLV (USA)	Short-term value: 3500 mg/m <sup>3</sup> , 1000 ppm Long-term value: 1760 mg/m <sup>3</sup> , 500 ppm

**71-43-2 Benzene (0,001%)**

MAK (Germany)	vgl. Abschn. XIII
MAK (TRGS 900) (Germany)	3,25 mg/m <sup>3</sup> , 1 ppm H, TRK; TRGS 901-15
TRK (TRGS 900) (Germany)	3,2 mg/m <sup>3</sup> , 1 ppm
PEL (USA)	Short-term value: 15* mg/m <sup>3</sup> , 5* ppm Long-term value: 3* mg/m <sup>3</sup> , 1* ppm *table Z-2 for exclusions in 29CFR1910,1028(d)
REL (USA)	Short-term value: 1 ppm Long-term value: 0,1 ppm See Pocket Guide App. A
TLV (USA)	Short-term value: 8 mg/m <sup>3</sup> , 2,5 ppm Long-term value: 1,6 mg/m <sup>3</sup> , 0,5 ppm Skin; BEI

**Ingredients with biological limit values:****110-54-3 n-Hexane (65,0%)**

BGW (Germany)	5 mg/l U b
BEI (USA)	2,5-Hexandion plus 4,5-Dihydroxy-2-hexanon 0,4 mg/L urine end of shift at end of workweek 2,5-Hexanedione without hydrolysis

**71-43-2 Benzene (0,001%)**

BEI (USA)	25 µg/g creatinine urine end of shift Parameter S-Phenylmercapturic acid (background)
	500 µg/g creatinine urine end of shift t,t-Muconic acid (background)

**Additional information:**

No data

**8.2 Exposure controls****Personal protective equipment****General protective and hygienic measures**

The usual precautionary measures should be adhered to in handling the chemicals.  
Keep away from foodstuffs, beverages and food.  
Instantly remove any soiled and impregnated garments.  
Wash hands during breaks and at the end of the work.  
Do not inhale dust / smoke / mist.  
Avoid contact with the skin.  
Avoid contact with the eyes and skin.  
Maintain an ergonomically appropriate working environment.  
Use breathing protection with high concentrations.  
Check protective gloves prior to each use for their proper condition.  
The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.  
Impervious gloves  
Not determined  
Safety glasses  
Face protection

**Breathing equipment:****Protection of hands:****Material of gloves****Penetration time of glove material****Eye protection:**(Contd. on page 4)  
DE/E

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Body protection: Protective work clothing.

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**SECTION 9: Physical and chemical properties****9.1 Information on basic physical and chemical properties****General Information****Appearance:**

Form: Liquid  
 Colour: Colourless  
 Smell: Not determined  
 Odour threshold: Not determined.

pH-value: Not determined.

**Change in condition**

Melting point/Melting range: -95 °C  
 Boiling point/Boiling range: 65-70 °C  
 Sublimation temperature / start: Not determined

Flash point: < -23 °C  
 Inflammability (solid, gaseous): Not determined.  
 Ignition temperature: 240 °C  
 Decomposition temperature: Not determined  
 Self-inflammability: Product is not selfigniting.

**Critical values for explosion:**

Lower: 1,2 Vol %  
 Upper: 7,7 Vol %

Steam pressure at 20 °C: 160 hPa  
 Density at 20 °C: 0,67 g/cm<sup>3</sup>

Relative density: Not determined.

Vapour density: Not determined.

Evaporation rate: Not determined.

**Solubility in / Miscibility with**

Water: Not miscible or difficult to mix

Partition coefficient (n-octanol/water): Not determined.

**Viscosity:**

dynamic: Not determined.

kinematic: Not determined.

**Solvent content:**

Organic solvents: 65,0 %

9.2 Other information: No further relevant information available.

**SECTION 10: Stability and reactivity****10.1 Reactivity**

No information known.

**10.2 Chemical stability**

Stable under recommended storage conditions.

**Thermal decomposition / conditions to be avoided:**

No decomposition if used and stored according to specifications.

**10.3 Possibility of hazardous reactions**

Reacts with strong oxidizing agents

**10.5 Incompatible materials:**

Oxidizing agents

10.6 Hazardous decomposition products: Carbon monoxide and carbon dioxide

**SECTION 11: Toxicological information****11.1 Information on toxicological effects**

Acute toxicity: The Registry of Toxic Effects of Chemical Substances (RTECS) contains acute toxicity data for components in this product.

**LD/LC50 values that are relevant for classification:****110-54-3 n-Hexane**

Oral LD50 15840 mg/kg (rat)

Inhalative LC50/4H 48000 ppm/4H (rat)

**71-43-2 Benzene**

Oral LD50 930 mg/kg (rat)

**Skin irritation or corrosion:**

Causes skin irritation.

**Eye irritation or corrosion:**

May cause irritation

**Sensitization:**

No sensitizing effect known.

**Germ cell mutagenicity:**

The Registry of Toxic Effects of Chemical Substances (RTECS) contains mutation data for components in this product.

**Carcinogenicity:**

EPA-II: Inadequate information to assess carcinogenic potential.  
 This product contains a substance or substances listed as a carcinogen by one or more of the following agencies: IARC, NTP, OSHA, ACGIH and EPA. Since this product contains <0.1% of the substance/ substances, the cancer warning has been omitted.  
 The Registry of Toxic Effects of Chemical Substances (RTECS) contains tumorigenic and/or carcinogenic and/ or neoplastic data for this product.

**Reproductive toxicity:**Suspected of damaging fertility or the unborn child.  
The Registry of Toxic Effects of Chemical Substances (RTECS) contains reproductive data for components in this product.**Specific target organ system toxicity - repeated exposure:**

May cause damage to the peripheral nervous system, the lung, the kidneys, the liver, the reproductive system and the brain through prolonged or repeated exposure. Route of exposure: Inhalative.

**Specific target organ system toxicity - single exposure:**

May cause drowsiness or dizziness.

May be fatal if swallowed and enters airways.

**Aspiration hazard:**

The Registry of Toxic Effects of Chemical Substances (RTECS) contains multiple dose toxicity data for components in this product.

**Experience with humans:**

To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.  
 The product shows the following dangers according to the calculation method of the General EC Classification Guidelines for Preparations as issued in the latest version:  
 Irritant

**SECTION 12: Ecological information****12.1 Toxicity**

Aquatic toxicity: No further relevant information available.

12.2 Persistence and degradability: No further relevant information available.

12.3 Bioaccumulative potential: No further relevant information available.

12.4 Mobility in soil: No further relevant information available.

(Contd. on page 5)  
DE/E

Trade name **Hexanes, mixed isomers, ACS**

(Contd. of page 4)

**Additional ecological information:**  
**General notes:**

Do not allow product to reach ground water, water bodies or sewage system.  
Do not allow material to be released to the environment without proper governmental permits.  
Water hazard class 2 (Self-assessment): hazardous for water.  
Danger to drinking water if even small quantities leak into soil.  
Also poisonous for fish and plankton in water bodies.  
Toxic to aquatic life.  
May cause long lasting harmful effects to aquatic life.  
Avoid transfer into the environment.

**12.5 Results of PBT and vPvB assessment****PBT:** Not applicable.**vPvB:** Not applicable.**12.6 Other adverse effects** No further relevant information available.**SECTION 13: Disposal considerations****13.1 Waste treatment methods****Recommendation**

Hand over to disposers of hazardous waste.  
Must be specially treated under adherence to official regulations.  
Consult state, local or national regulations for proper disposal.

**Uncleaned packagings:****Recommendation:**

Disposal must be made according to official regulations.

**SECTION 14: Transport information****UN-Number**  
**ADR, IMDG, IATA**

UN1208

**14.2 UN proper shipping name**

**ADR** 1208 HEXANES  
**IMDG** HEXANES, MARINE POLLUTANT  
**IATA** HEXANES

**14.3 Transport hazard class(es)**

**ADR**



**Class** 3 (F1) Flammable liquids.  
**Label** 3  
**IMDG**



**Class** 3 Flammable liquids.  
**Label** 3  
**IATA**



**Class** 3 Flammable liquids.  
**Label** 3

**Packing group**  
**ADR, IMDG, IATA**

II

**14.5 Environmental hazards:****Marine pollutant:**

Product contains environmentally hazardous substances: n-Hexane, anhydrous, 3-Methylpentane  
Symbol (fish and tree)

**14.6 Special precautions for user****Kemler Number:****EMS Number:**

Warning: Flammable liquids.  
33  
F-E,S-D

**14.7 Transport in bulk according to Annex II of MARPOL73/78 and the IBC****Code** Not applicable.**Transport/Additional information:**

**ADR**

**Excepted quantities (EQ):** E2  
**Limited quantities (LQ)** 1L  
**Transport category** 2  
**Tunnel restriction code** D/E

**UN "Model Regulation":** UN1208, HEXANES, 3, II**SECTION 15: Regulatory information****15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture****Australian Inventory of Chemical Substances**

All ingredients are listed.

**Standard for the Uniform Scheduling of Drugs and Poisons**

71-43-2 | Benzene

S7

**National regulations****Information about limitation of use:**

Employment restrictions concerning young persons must be observed.  
Employment restrictions concerning women of child-bearing age must be observed.  
For use only by technically qualified individuals.

**Classification according to VbF:****Technical instructions (air):**

Class	Share in %
I	65.0

**Water hazard class:****Other regulations, limitations and prohibitive regulations**

Water hazard class 2 (Self-assessment): hazardous for water.

**ELINCS (European List of Notified Chemical Substances)**

None of the ingredients is listed.

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DE/E

**Safety data sheet**  
according to 1907/2006/EC, Article 31

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**Substances of very high concern (SVHC) according to REACH, Article 57**

None of the ingredients are listed.

**REACH - Pre-registered substances**

All ingredients are listed.

**15.2 Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.**SECTION 16: Other information**

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

**Relevant phrases**

H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H336	May cause drowsiness or dizziness.
H361f	Suspected of damaging fertility.
H373	May cause damage to the peripheral nervous system, the lung, the kidneys, the liver, the reproductive system and the brain through prolonged or repeated exposure. Route of exposure: Inhalative.
H411	Toxic to aquatic life with long lasting effects.
R11	Highly flammable.
R36/37/38	Irritating to eyes, respiratory system and skin.
R38	Irritating to skin.
R48/20	Harmful: danger of serious damage to health by prolonged exposure through inhalation.
R51/53	Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.
R62	Possible risk of impaired fertility.
R65	Harmful: may cause lung damage if swallowed.
R67	Vapours may cause drowsiness and dizziness.

**Department issuing data specification sheet:****Abbreviations and acronyms:**

Health, Safety and Environmental Department.  
 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  
 VbF: Verordnung über brennbare Flüssigkeiten, Österreich (Ordinance on the storage of combustible liquids, Austria)  
 LC50: Lethal concentration, 50 percent  
 LD50: Lethal dose, 50 percent

DE/E