Safety data sheet
n-Heptane

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

1.1. Product identifier
Product name
n-Heptane
EC No (from EINECS): 205-563-8
CAS No: 142-82-5
Index-Nr. 601-008-00-2
Chemical formula C7H16
REACH Registration number:
01-2119457603-38

1.2. Relevant identified uses of the substance or mixture and uses advised against
Relevant identified uses
Industrial and professional. Perform risk assessment prior to use.
Uses advised against
Consumer use.

1.3. Details of the supplier of the safety data sheet
Company identification
BOC, Priestley Road, Worsley, Manchester M28 2UT
E-Mail Address ReachSDS@boc.com

1.4. Emergency telephone number
Emergency phone numbers (24h): 0800 111 333

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification acc. to Regulation (EC) No 1272/2008/EC (CLP/GHS)
Flammable liquid: Flam. Liq. 2 – Highly flammable liquid and vapour.
Asp. Tox. 1 - May be fatal if swallowed and enters airways.
Skin Irrit. 2 - Causes skin irritation.
STOT SE 3 - May cause drowsiness or dizziness.
Aquatic Acute 1 - Very toxic to aquatic life.
Aquatic Chronic 1 - Very toxic to aquatic life with long lasting effects.

Classification acc. to Directive 67/548/EEC & 1999/45/EC:
F; R11 **|** Xn; R65 **|** Xi; R38 **|** R67 **|** N; R50/53
Highly flammable.
Irritating to skin.
Very toxic to aquatic organisms, may cause long term adverse effects in the aquatic environment.
Harmful: may cause lung damage if swallowed.
Vapours may cause drowsiness and dizziness.

2.2. Label elements
- Labelling Pictograms

- Signal word

Danger

- **Hazard Statements**

H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation
H336	May cause drowsiness or dizziness.
H410	Very toxic to aquatic life with long lasting effects.

- **Precautionary Statements**

Precautionary Statement Prevention

P210	Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P233	Keep container tightly closed.
P240	Ground / bond container and receiving equipment.
P241	Use explosion-proof electrical, ventilating, and lighting equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P261	Avoid breathing mist / vapours.
P271	Use only outdoors or in a well-ventilated area.
P273	Avoid release to the environment.
P280	Wear protective gloves and eye / face protection.

Precautionary Statement Response

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
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P312	Call a POISON CENTER or doctor/physician if you feel unwell.
P331	Do NOT induce vomiting.
P370 + P378	In case of fire: Use water fog, foam, dry chemical or carbon dioxide (CO2) for extinction.
P391	Collect spillage.

Precautionary Statement Storage

P403 + P233+ P235	Store in a well-ventilated place. Keep container tightly closed. Keep cool.
P405	Store locked up.

Precautionary Statement Disposal

P501	Dispose of contents and container in accordance with local regulations.

2.3. Other hazards

SECTION 3: Composition/information on ingredients

Substance / Mixture: Substance.

3.1. Substances
n-Heptane
EC No (from EINECS): 205-563-8
CAS No: 142-82-5
Index-Nr. 601-008-00-2
Chemical formula C7H16
REACH Registration number:
01-2119457603-38

Contains no other components or impurities which will influence the classification of the product.

3.2. Mixtures
Not applicable.

SECTION 4: First aid measures

4.1. Description of first aid measures
First Aid General Information:
Remove victim to uncontaminated area wearing self contained breathing apparatus. Keep victim warm and rested. Call a doctor. Apply artificial respiration if breathing stopped.
First Aid Inhalation:
Remove victim to uncontaminated area wearing self contained breathing apparatus. Keep victim warm and rested. Call a doctor. Apply artificial respiration if breathing stopped.
First Aid Skin / Eye:
For liquid spillage - flush with water for at least 15 minutes. Remove contaminated clothing. Drench affected area with water for at least 15 minutes. Immediately flush eyes thoroughly with water for at least 15 minutes. Obtain medical assistance.
First Aid Ingestion:
If victim is conscious: Rinse mouth out with plenty of water.
Let victim drink water as much as possible in small sips
Do NOT induce vomiting.
Get immediate medical advice/attention.
4.2. Most important symptoms and effects, both acute and delayed
Causes skin and eye irritation . Possible symptoms are irritation of the mucous membranes, dry cough and respiratory difficulty. Symptoms may include dizziness, headache, nausea and loss of co-ordination Suitable first-aid treatment should be immediately available. Seek medical advice before using product. May result in pulmonary oedema.

4.3. Indication of any immediate medical attention and special treatment needed
Obtain medical assistance.
Recommendations to physicians: Provide oxygen.

SECTION 5: Fire fighting measures

5.1. Extinguishing media
Suitable extinguishing media
Dry powder.. Carbon dioxide. Alcohol-resistant foam. Use water spray or fog to control fire fumes.
Unsuitable extinguishing media
Do not use a solid water stream.

5.2. Special hazards arising from the substance or mixture
Specific hazards
Exposure to fire may cause containers to rupture/explode.
Hazardous combustion products
If involved in a fire the following toxic and/or corrosive fumes may be produced by thermal decomposition: Carbon dioxide and Carbon monoxide

5.3. Advice for fire-fighters
Specific methods
If possible, stop flow of product. If leaking do not extinguish a flame unless absolutely necessary. Spontaneous/explosive re-ignition may occur. Extinguish any other fire. Move container away or cool with water from a protected position. Prevent water used in emergency cases from entering sewers and drainage systems.
Special protective equipment for fire-fighters
Normal firefighters' equipment consists of an appropriate SCBA (open-circuit positive pressure compressed air type) in combination with fire kit. Equipment and clothing to the following standards will provide a suitable level of protection for firefighters.
Guideline:
EN 469:2005: Protective clothing for firefighters. Performance requirements for protective clothing for firefighting., EN 137 Respiratory protective devices — Self-contained open-circuit compressed air breathing apparatus with full face mask — Requirements, testing, marking., EN 15090 Footwear for firefighters., EN 443 Helmets for fire fighting in buildings and other structures., EN 659 Protective gloves for firefighters.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures
Evacuate area. Use self-contained breathing apparatus and chemically protective clothing. Ensure adequate air ventilation. Eliminate ignition sources. Consider the risk of potentially explosive atmospheres. Monitor concentration of released product. Prevent from entering sewers, basements and workpits, or any place where its accumulation can be dangerous.

6.2. Environmental precautions
Try to stop release. Reduce vapour with fog or fine water spray.

6.3. Methods and material for containment and cleaning up
Ventilate area. Keep away from ignition sources (including static discharges). Evacuate area. Prevent evaporation by covering with foam. Absorb excess liquid spillage on inorganic adsorbent material such as fine sand, brick dust etc. Place spent adsorbent in sealed packages and contact specialist waste disposal contractor.

6.4. Reference to other sections
See also sections 8 and 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling
Only experienced and properly instructed persons should use this product. The substance must be handled in accordance with good industrial hygiene and safety procedures. Use only properly specified equipment which is suitable for this product, its supply pressure and temperature. Contact your supplier if in doubt. Avoid exposure, obtain special instructions before use. Take precautionary measures against static discharges. Ensure equipment is adequately earthed. Purge air from system before introducing product. Keep away from ignition sources (including static discharges). Do not smoke while handling product. Assess the risk of a potentially explosive atmosphere and use explosion-proof equipment. Use only non-sparking tools. Ensure the complete system has been (or is regularly) checked for leaks before use. Installation of a cross purge assembly between the container and the regulator is recommended. Purge system with dry inert gas (e.g. helium or nitrogen) before product is introduced and when system is placed out of service. Avoid suckback of water, acid and alkalis. Refer to supplier's handling instructions. Do not allow backfeed into the container. Protect containers from physical damage; do not drag, roll, slide or drop. When moving containers, even for short distances, use appropriate equipment e.g. trolley, hand truck, fork truck etc. Leave valve protection caps in place until the container has been secured against either a wall or bench or placed in a container stand and is ready for use. If user experiences any difficulty operating container valve discontinue use and contact supplier. Never attempt to repair or modify container valves or safety relief devices. Damaged valves should be reported immediately to the supplier. Keep container valve outlets clean and free from contaminates particularly oil and water. Replace valve outlet caps or

plugs and container caps where supplied as soon as container is disconnected from equipment. Close container valve after each use and when empty, even if still connected to equipment. Never attempt to transfer product from one container to another. Never use direct flame or electrical heating devices to raise the pressure of a container. Do not remove or deface labels provided by the supplier for the identification of the container contents.

7.2. Conditions for safe storage, including any incompatibilities
Segregate from oxidant gases and other oxidants in store. Keep container below 50°C in a well ventilated place. Secure cylinders to prevent them from falling. Observe all regulations and local requirements regarding storage of containers. Cylinders should be stored in the vertical position and properly secured to prevent falling over. Stored containers should be periodically checked for general conditions and leakage. Container valve guards or caps should be in place. Store containers in location free from fire risk and away from sources of heat and ignition. Keep away from combustible materials. All electrical equipment in the storage areas should be compatible with the risk of potentially explosive atmosphere. Containers should not be stored in conditions likely to encourage corrosion.

7.3. Specific end use(s)
None.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters
Exposure limit value

Value type	Value	Note
Great Britain - LTEL	500 ppm	EH 40/07

Derived No Effect Levels

Type	Exposure	Value	Population	Effects
DNEL	Long term Dermal	300 mg/kg bw/day	Workers	Systemic
DNEL	Long term Inhalation	2085 mg/m³	Workers	Systemic

Predicted No Effect Concentrations

Type	Compartment Detail	Value
PNEC	Fresh water	0,03 mg/L
PNEC	Marine water	0,03 mg/L
PNEC	Fresh water sediment	4,4 mg/kg
PNEC	Marine sediment	4,4 mg/kg
PNEC	Soil	1,8 mg/kg

8.2. Exposure controls
Appropriate engineering controls
A risk assessment should be conducted and documented in each work area to assess the risks related to the use of the product and to select the PPE that matches the relevant risk. The following recommendations should be considered. Gas detectors should be used when toxic quantities may be released. Gas detectors should be used when quantities of flammable gases/vapours may be released. Consider work permit system e.g. for maintenance activities. Systems under pressure should be regularly checked for leakages. Provide adequate general or local ventilation.
Personal protective equipment
Eye and face protection
Protect eyes, face and skin from contact with product. Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Wear a face-shield when transfilling and breaking transfer connections. Safety eyewear, goggles or face-shield to EN166 should be used to avoid exposure to liquid splashes. Wear eye protection to EN 166 when using the product. Full-face mask recommended
Guideline:
EN 136 Respiratory protective devices. Full face masks. Requirements, testing, marking
Skin protection
Hand protection
Advice: Wear working gloves and safety shoes while handling containers., Chemically resistant gloves complying with EN 374 should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Guideline: EN 388 Protective gloves. EN 374-1/2/3 Protective gloves against chemicals and micro-organisms.

Body protection
Protect eyes, face and skin from contact with product. Keep suitable chemically resistant protective clothing readily available for emergency use. Personal protective equipment for the body should be selected based on the task being performed and the risks involved.
Guideline:
EN 943: Protective clothing against liquid and gaseous chemicals, including liquid aerosols and solid particles.
Other protection
Wear flame resistant/retardant clothing. Take precautionary measures against static discharges. Wear working gloves and safety shoes while handling containers. EN ISO 20345 Personal protective equipment - Safety footwear. ISO/TR 2801:2007 Clothing for protection against heat and flame -- General recommendations for selection, care and use of protective clothing.
Respiratory protection
Keep self contained breathing apparatus readily available for emergency use., Use SCBA in the event of high concentrations, The selection of the Respiratory Protective Device (RPD) must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected RPD., When a risk assessment shows that air-purifying respirators are appropriate then they may be used as a back-up to engineering controls. If the respirator is the sole means of protection use a full face supplied air respirator.
Guideline:
EN 136 Respiratory protective devices. Full face masks. Requirements, testing, marking

Material:
Filter ABEK

Guideline:
EN 14387: Respiratory protective devices. Gas filter(s) and combined filter(s). Requirements, testing, marking.

Self-contained breathing apparatus (SCBA)

Guideline:
EN 137 Respiratory protective devices — Self-contained open circuit compressed air breathing apparatus with full face mask — Requirements, testing, marking.
Thermal hazards
Not applicable
Environmental Exposure Controls
Specific risk management measures are not required beyond good industrial hygiene and safety procedures. Refer to local regulations for restriction of emissions to the atmosphere. See section 13 for specific methods for waste gas treatment.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties
General information
Appearance/Colour:
Odour: Petroleum-like odour, almost odourless.
Odour threshold:
Odour threshold is subjective and inadequate to warn for over exposure.
Melting point: -91°C
Boiling point: 98,4°C
Flash point: -4°C
Evaporation rate: No data available.
Flammability range: 1,1 %(V) – 7 %(V)
Vapour Pressure 20 °C: 53,3 hPa
Relative density, gas (Air=1): 3,5
Solubility in water: Negligible
Partition coefficient: n-octanol/water: 4,66
Autoignition temperature: 203,85°C
Molecular weight: 100,23 g/mol
Critical temperature: No data available.
Relative density, liquid (Water=1): 0,7

9.2. Other information
Gas/vapour heavier than air. May accumulate in confined spaces, particularly at or below ground level.

SECTION 10: Stability and reactivity

10.1. Reactivity
No reactivity hazard other than the effects described in sub-sections below.

10.2. Chemical stability
Stable under normal conditions.

10.3. Possibility of hazardous reactions
Can form potentially explosive atmosphere in air. May react violently with oxidants.

10.4. Conditions to avoid
Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

10.5. Incompatible materials
Air, Oxidiser

10.6. Hazardous decomposition products
Under normal conditions of storage and use, hazardous decomposition products should not be produced. If involved in a fire the following toxic and/or corrosive fumes may be produced by thermal decomposition:
Carbon dioxide and Carbon monoxide

SECTION 11: Toxicological information

11.1. Information on toxicological effects
Acute inhalation toxicity
Value: LC50
Species: Rat
Method: OECD Test Guideline 403
Exposure time: 4 h
Value in non-standard unit: 29,29 mg/l
May result in pulmonary oedema
Acute oral toxicity
Value: LD50
Species: Rat
Method: OECD Test Guideline 401
Value in non-standard unit: >5000 mg/kg
Read across.
Acute dermal toxicity
Value: LD50
Species: Rabbit
Method: OECD Test Guideline 402
Value in non-standard unit: >2000 mg/kg
Read across.
Skin irritation
Irritating to skin.
Eye irritation
Irritating to eyes.
Sensitization
Not sensitising.
Read across.
Repeated dose toxicity
Species: Rat
Route of application: Inhalation
Exposure time: 16 weeks
Value type: NOAEC
Value: 12470 mg/m³ air
Genetic toxicity in vitro
Negative
Genetic toxicity in vivo
No data available.
Assessment carcinogenicity
No data available.
Toxicity to reproduction/fertility
Species: Rat
Route of application: Inhalation
Value type: NOAEL
Value: 9000 ppm

Value type: NOAEL F1
Value: 3000 ppm

Value type: NOAEL F2
Value: 3000 ppm

Method: OECD Test Guideline 416
Test substance: Read across
Developmental toxicity/teratogenicity
Species: Mouse
Route of application: Inhalation
Value type: NOAEL (maternal)
Value: 900 ppm

Value type: NOAEL (developmental)
Value: 3000 ppm

Value type: LOAEL
Value: 9000 ppm

Method: OECD Test Guideline 414
Test substance: Read across
Specific Target Organ Toxicity (STOT) - Single Exposure
May cause drowsiness or dizziness.
Specific Target Organ Toxicity (STOT) - Repeated Exposure
No data available.
Aspiration hazard
Aspirated material may produce fatal lung injury.

SECTION 12: Ecological information

12.1. Toxicity
Acute and prolonged toxicity fish
Species: Rainbow trout (Oncorhynchus mykiss)
Exposure time: 28d

Method: QSAR
Value type: NOELR
Value in standard unit mg/l: 1,284

Species: Rainbow trout (Oncorhynchus mykiss)
Exposure time: 96h
Method: QSAR
Value type: LL50
Value in standard unit mg/l: 5,738
Toxicity aquatic invertebrates
Species: Water flea (Daphnia magna)
Exposure time: 48h
Value type: EC50
Value in standard unit mg/l: 1,5

Species: Water flea (Daphnia magna)
Exposure time: 21d
Method: OECD Test Guideline 211
Value type: NOELR
Value in standard unit mg/l: 1
Read across

Toxicity aquatic plants
Species: Algae
Exposure time: 72h
Value type: EL50
Value in standard unit mg/l: 4,338
Method: QSAR

12.2. Persistence and degradability
Compartment: Water
Test duration: 10d
Degradation: 70%
The overall results suggest that it would meet the criteria for ready biodegradation.

12.3. Bioaccumulative potential
Log Pow: 4,66
Has potential to bioaccumulate.

12.4. Mobility in soil
n-Heptane is calculated by the Level I fugacity-based Equilibrium Partitioning model to partition 100% into the air phase.

12.5. Results of PBT and vPvB assessment
Not classified as PBT or vPvB.

12.6. Other adverse effects
Very toxic to aquatic life with long lasting effects. Avoid release to the environment.

SECTION 13: Disposal considerations

13.1. Waste treatment methods
Avoid release to the environment. Do not discharge into any place where its accumulation could be dangerous. Contact supplier if guidance is required. Toxic and corrosive gases formed during combustion should be scrubbed before discharge to atmosphere. Do not discharge into areas where there is a risk of forming an explosive mixture with air. Waste gas should be flared through a suitable burner with flash back arrestor.

SECTION 14: Transport information

ADR/RID

14.1. UN number
1206

14.2. UN proper shipping name
Heptanes

14.3. Transport hazard class(es)
Class: 3
Classification Code: F1
Labels: 3
Hazard number: 33
Tunnel restriction code: (D/E)
Emergency Action Code: 3YE

14.4. Packing group (Packing Instruction)
II

14.5. Environmental hazards
Environmentally hazardous.

14.6. Special precautions for user
None.

IMDG

14.1. UN number
1206

14.2. UN proper shipping name
Heptanes

14.3. Transport hazard class(es)
Class: 3
Labels: 3
EmS: F-E, S-D

14.4. Packing group (Packing Instruction)
II

14.5. Environmental hazards
Environmentally hazardous.

14.6. Special precautions for user
Immiscible with water. Irritating to skin, eyes and mucous membranes.

14.7. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code
Substance name: HEPTANE (ALL ISOMERS)
Ship type required: 2
Pollution category: X

IATA

14.1. UN number
1206

14.2. UN proper shipping name
Heptanes

14.3. Transport hazard class(es)
Class: 3

14.4. Packing group (Packing Instruction)
Passenger Aircraft: Permitted for transport
Cargo Aircraft: Permitted for transport

14.5. Environmental hazards
None.

14.6. Special precautions for user

None.

Other transport information
Avoid transport on vehicles where the load space is not separated from the driver's compartment. Ensure vehicle driver is aware of the potential hazards of the load and knows what to do in the event of an accident or an emergency. Before transporting product containers ensure that they are firmly secured. Ensure that the container valve is closed and not leaking. Ensure that the valve outlet cap nut or plug (where provided) is correctly fitted. Ensure that the valve protection device (where provided) is correctly fitted. Ensure adequate ventilation. Ensure compliance with applicable regulations.

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture
Seveso Directive 96/82/EC: Covered

Other regulations
Dangerous Substances and Explosive Atmospheres Regulations (DSEAR 2002 No. 2776)
Management of Health and Safety at Work Regulations (1999 No. 3242)
The Regulatory Reform (Fire Safety) Order 2005 (2005 No. 1541)
Control of Substances Hazardous to Health Regulations (COSHH, 2002 No. 2677)
Equipment and Protective Systems Intended for Use in Potentially Explosive Atmospheres Regulations (EPS, 1996 No. 192)
Provision and Use of Work Equipment Regulations (PUWER, 1998 No. 2306)
Personal Protective Equipment Regulations (1992 No. 2966)
Control of Major Accident Hazards Regulations (COMAH, 1999 No. 743)
Chemical Hazards Information and Packaging for Supply (CHIP, 1994 No. 3247)
Pressure Systems Safety Regulations (PER, 2000 No. 128)
This Safety Data Sheet has been produced to comply with Regulation (EU) 453/2010.

15.2. Chemical safety assessment
A CSA has been carried out.

SECTION 16: Other information

Ensure operators understand the flammability hazard. Ensure operators understand the toxicity hazard. Users of breathing apparatus must be trained. Before using this product in any new process or experiment, a thorough material compatibility and safety study should be carried out.

Advice
Whilst proper care has been taken in the preparation of this document, no liability for injury or damage resulting from its use can be accepted. Details given in this document are believed to be correct at the time of going to press.

Further information
Note:
When using this document care should be taken, as the decimal sign and its position complies with rules for the structure and drafting of international standards, and is a comma on the line.
As an example 2,000 is two (to three decimal places) and not two thousand, whilst 1.000 is one thousand and not one (to three decimal places).

References
Various sources of data have been used in the compilation of this SDS; they include but are not exclusive to:

European Chemical Agency: Guidance on the Compilation of Safety Data Sheets.
European Chemical Agency: Information on Registered Substances http://apps.echa.europa.eu/registered/registered-sub.aspx#search
European Industrial Gases Association (EIGA) Doc. 169/11 Classification and Labelling guide.
ISO 10156:2010 Gases and gas mixtures -- Determination of fire potential and oxidizing ability for the selection of cylinder valve outlets.
International Programme on Chemical Safety (http://www.inchem.org/)
Matheson Gas Data Book, 7th Edition.
National Institute for Standards and Technology (NIST) Standard Reference Database Number 69
The ESIS (European chemical Substances 5 Information System) platform of the former European Chemicals Bureau (ECB) ESIS (http://ecb.jrc.ec.europa.eu/esis/).
The European Chemical Industry Council (CEFIC) ERICards.
United States of America's National Library of Medicine's toxicology data network TOXNET (http://toxnet.nlm.nih.gov/index.html)
Agency for Toxic Substances and Diseases Registry (ATSDR) (http://www.atsdr.cdc.gov/)
Threshold Limit Values (TLV) from the American Conference of Governmental Industrial Hygienists (ACGIH).
Substance specific information from suppliers.
EH40 (as amended) Workplace exposure limits.

End of document