

Safety Data Sheet

acc. to OSHA HCS

Printing date 06/07/2024

Reviewed on 06/07/2024

1 Identification

- **Product identifier**
- **Trade name:** Aromatics by HPLC
QC Standard ASTM D6591
- **Article number:** HOU043
- **Details of the supplier of the safety data sheet**
- **Manufacturer/Supplier:**
Aqua Solutions, Inc.
6913 Highway 225
DEER PARK, TX 77536
USA
800-256-2586
- **Information department:**
Technical Coordinator
Sherman Nelson shermann@aquasolutions.org
- **Emergency telephone number:**
Chemtrec: 800-424-9300
Canutec: 613-996-6666



2 Hazard(s) identification

- **Classification of the substance or mixture**



GHS02 Flame

Flammable Liquids 2

H225 Highly flammable liquid and vapor.



GHS08 Health hazard

Aspiration Hazard 1

H304 May be fatal if swallowed and enters airways.



GHS07

Skin Irritation 2

H315 Causes skin irritation.

Specific Target Organ Toxicity - Single Exposure 3 H336 May cause drowsiness or dizziness.

- **Label elements**
- **GHS label elements** The product is classified and labeled according to the Globally Harmonized System (GHS).
- **Hazard pictograms**



GHS02



GHS07



GHS08

- **Signal word** *Danger*
- **Hazard-determining components of labeling:**
Cyclohexane
n-Heptane

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- **Hazard statements**

Highly flammable liquid and vapor.
 Causes skin irritation.
 May cause drowsiness or dizziness.
 May be fatal if swallowed and enters airways.

- **Precautionary statements**

Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
 Ground/bond container and receiving equipment.
 Use explosion-proof electrical/ventilating/lighting/equipment.
 Use only non-sparking tools.
 Take precautionary measures against static discharge.
 Avoid breathing dust/fume/gas/mist/vapors/spray
 Wash thoroughly after handling.
 Use only outdoors or in a well-ventilated area.
 Wear protective gloves/protective clothing/eye protection/face protection.
 If swallowed: Immediately call a poison center/doctor.
 Specific treatment (see on this label).
 Do NOT induce vomiting.
 If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
 Call a poison center/doctor if you feel unwell.
 Take off contaminated clothing and wash it before reuse.
 If skin irritation occurs: Get medical advice/attention.
 In case of fire: Use CO₂, powder or water spray to extinguish.
 Store in a well-ventilated place. Keep container tightly closed.
 Store in a well-ventilated place. Keep cool.
 Store locked up.
 Dispose of contents/container in accordance with local/regional/national/international regulations.

- **Classification system:**

- **NFPA ratings (scale 0 - 4)**



Health = 1
 Fire = 3
 Reactivity = 0

- **HMIS-ratings (scale 0 - 4)**



HEALTH 1 Health = 1
 FIRE 3 Fire = 3
 REACTIVITY 0 Reactivity = 0

- **Other hazards**

- **Results of PBT and vPvB assessment**

- **PBT:** Not applicable.

- **vPvB:**

Phenanthrene, 98%

3 Composition/information on ingredients

- **Chemical characterization: Mixtures**

- **Description:** Mixture of the substances listed below with nonhazardous additions.

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· Dangerous components:		
CAS: 110-82-7	Cyclohexane	64.136%
CAS: 95-47-6	o-Xylene	19.241%
CAS: 142-82-5	n-Heptane	15.682%
	Phenanthrene, 98%	0.3%
· Table of Nonhazardous Ingredients		
CAS: 90-12-0	1-methylnaphthalene	0.641%

4 First-aid measures

- **Description of first aid measures**
- **General information:** Immediately remove any clothing soiled by the product.
- **After inhalation:** In case of unconsciousness place patient stably in side position for transportation.
- **After skin contact:** Immediately wash with water and soap and rinse thoroughly.
- **After eye contact:** Rinse opened eye for several minutes under running water.
- **After swallowing:** If symptoms persist consult doctor.
- **Information for doctor:**
- **Most important symptoms and effects, both acute and delayed** No further relevant information available.
- **Indication of any immediate medical attention and special treatment needed**
No further relevant information available.

5 Fire-fighting measures

- **Extinguishing media**
- **Suitable extinguishing agents:**
CO₂, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
- **For safety reasons unsuitable extinguishing agents:** Water with full jet
- **Special hazards arising from the substance or mixture** No further relevant information available.
- **Advice for firefighters**
- **Protective equipment:** No special measures required.

* 6 Accidental release measures

- **Personal precautions, protective equipment and emergency procedures**
Wear protective equipment. Keep unprotected persons away.
- **Environmental precautions:**
Do not allow product to reach sewage system or any water course.
Inform respective authorities in case of seepage into water course or sewage system.
Do not allow to enter sewers/ surface or ground water.
- **Methods and material for containment and cleaning up:**
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
Dispose contaminated material as waste according to section 13.
Ensure adequate ventilation.
- **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 disposal information.

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· Protective Action Criteria for Chemicals

· PAC-1:		
CAS: 110-82-7	Cyclohexane	300 ppm
CAS: 142-82-5	n-Heptane	500 ppm
CAS: 90-12-0	1-methylnaphthalene	20 mg/m ³
	Phenanthrene, 98%	5.4 mg/m ³
· PAC-2:		
CAS: 110-82-7	Cyclohexane	1700* ppm
CAS: 142-82-5	n-Heptane	830 ppm
CAS: 90-12-0	1-methylnaphthalene	61 mg/m ³
	Phenanthrene, 98%	59 mg/m ³
· PAC-3:		
CAS: 110-82-7	Cyclohexane	10000** ppm
CAS: 142-82-5	n-Heptane	5000* ppm
CAS: 90-12-0	1-methylnaphthalene	360 mg/m ³
	Phenanthrene, 98%	360 mg/m ³

7 Handling and storage

· Handling:

· Precautions for safe handling

Ensure good ventilation/exhaustion at the workplace.

Prevent formation of aerosols.

· Information about protection against explosions and fires:

Keep ignition sources away - Do not smoke.

Protect against electrostatic charges.

· Conditions for safe storage, including any incompatibilities

· Storage:

· **Requirements to be met by storerooms and receptacles:** Store in a cool location.

· **Information about storage in one common storage facility:** Not required.

· Further information about storage conditions:

Keep receptacle tightly sealed.

Store in cool, dry conditions in well sealed receptacles.

· **Specific end use(s)** No further relevant information available.

8 Exposure controls/personal protection

· **Additional information about design of technical systems:** No further data; see section 7.

· Control parameters

· Components with limit values that require monitoring at the workplace:

CAS: 110-82-7 Cyclohexane	
PEL	Long-term value: 1050 mg/m ³ , 300 ppm
REL	Long-term value: 1050 mg/m ³ , 300 ppm
TLV	Long-term value: 100 ppm
BEI	

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CAS: 95-47-6 o-Xylene

PEL	Long-term value: 435 mg/m ³ , 100 ppm
REL	Short-term value: 655 mg/m ³ , 150 ppm Long-term value: 435 mg/m ³ , 100 ppm
TLV	Long-term value: 20 ppm BEI, A4

CAS: 142-82-5 n-Heptane

PEL	Long-term value: 2000 mg/m ³ , 500 ppm
REL	Long-term value: 350 mg/m ³ , 85 ppm Ceiling limit value: 1800* mg/m ³ , 440* ppm *15-min
TLV	Short-term value: 500 ppm Long-term value: 400 ppm

Phenanthrene, 98%

TWA	Short-term value: 0.2 mg/m ³
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· **Ingredients with biological limit values:****CAS: 110-82-7 Cyclohexane**

BEI	NIC-50 mg/g creatinine LD50 Intraperitoneal: - Time: end of shift at end of workweek LD50: NIC-1.2-Cyclohexanediol (nonspecific)
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CAS: 95-47-6 o-Xylene

BEI	1.5 g/g creatinine LD50 Intraperitoneal: urine Time: end of shift LD50: Methylhippuric acids
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· **Additional information:** The lists that were valid during the creation were used as basis.

· **Exposure controls**· **Personal protective equipment:**· **General protective and hygienic measures:**

- Keep away from foodstuffs, beverages and feed.
- Immediately remove all soiled and contaminated clothing.
- Wash hands before breaks and at the end of work.
- Avoid contact with the skin.
- Avoid contact with the eyes and skin.

· **Breathing equipment:**

In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.

· **Protection of hands:**

Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.

Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

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- **Material of gloves**

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. As the product is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.

- **Penetration time of glove material**

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

- **Eye protection:**



Tightly sealed goggles

- **Body protection:** Protective work clothing

9 Physical and chemical properties

- **Information on basic physical and chemical properties**

- **General Information**

- **Appearance:**

Form:	Liquid
Color:	Clear
Odor:	Distinct
Odor threshold:	Not determined.

- **pH-value:** Not determined.

- **Change in condition**

Melting point/Melting range:	Undetermined.
Boiling point/Boiling range:	81 °C (177.8 °F)

- **Flash point:** -18 °C (-0.4 °F)

- **Flammability (solid, gaseous):** Highly flammable.

- **Auto igniting:** 215 °C (419 °F)

- **Decomposition temperature:** Not determined.

- **Ignition temperature:** Product is not selfigniting.

- **Danger of explosion:** Product is not explosive. However, formation of explosive air/vapor mixtures are possible.

- **Explosion limits:**

Lower:	1.1 Vol %
Upper:	8.3 Vol %

- **Vapor pressure at 20 °C (68 °F):** 104 hPa (78 mm Hg)

- **Vapor pressure at 50 °C (122 °F):** 335 hPa (251.3 mm Hg)

- **Density at 20 °C (68 °F):** 0.78435 g/cm³ (6.5454 lbs/gal)

- **Relative density** Not determined.

- **Vapor density** Not determined.

- **Evaporation rate** Not determined.

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- | | |
|---|--|
| · 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: | 99.1 % |
| VOC content: | 99.06 % |
| | 777.0 g/l / 6.48 lb/gal |
| · Solids content: | 0.0 % |
| · Other information | No further relevant information available. |

10 Stability and reactivity

- **Reactivity** No further relevant information available.
- **Chemical stability**
- **Thermal decomposition / conditions to be avoided:** No decomposition if used according to specifications.
- **Possibility of hazardous reactions** No dangerous reactions known.
- **Conditions to avoid** No further relevant information available.
- **Incompatible materials:** No further relevant information available.
- **Hazardous decomposition products:** No dangerous decomposition products known.

11 Toxicological information

- **Information on toxicological effects**
- **Acute toxicity:**

- **LD/LC50 values that are relevant for classification:**

ATE (Acute Toxicity Estimate)

Dermal	LD50	5,717 mg/kg
Inhalative	LC50/4h	57.2 mg/l

- **Primary irritant effect:**
- **on the skin:** Irritant to skin and mucous membranes.
- **on the eye:** No irritating effect.
- **Sensitization:** No sensitizing effects known.
- **Additional toxicological information:**
The product shows the following dangers according to internally approved calculation methods for preparations:
Irritant

- **Carcinogenic categories**

- **IARC (International Agency for Research on Cancer)**

CAS: 95-47-6	o-Xylene	3
	Phenanthrene, 98%	3

- **NTP (National Toxicology Program)**

Phenanthrene, 98%		R
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· **OSHA-Ca (Occupational Safety & Health Administration)**

None of the ingredients is listed.

12 Ecological information

- **Toxicity**
- **Aquatic toxicity:** No further relevant information available.
- **Persistence and degradability** No further relevant information available.
- **Behavior in environmental systems:**
- **Bioaccumulative potential** No further relevant information available.
- **Mobility in soil** No further relevant information available.
- **Additional ecological information:**
- **General notes:**
 Water hazard class 2 (Self-assessment): hazardous for water
 Do not allow product to reach ground water, water course or sewage system.
 Danger to drinking water if even small quantities leak into the ground.
- **Results of PBT and vPvB assessment**
- **PBT:** Not applicable.

· **vPvB:**

Phenanthrene, 98%

- **Other adverse effects** No further relevant information available.

13 Disposal considerations

- **Waste treatment methods**
- **Recommendation:**
 Must not be disposed of together with household garbage. Do not allow product to reach sewage system.
- **Uncleaned packagings:**
- **Recommendation:** Disposal must be made according to official regulations.

14 Transport information

- **UN-Number**
- **DOT, IMDG, IATA** UN1993
- **UN proper shipping name**
- **DOT** Flammable liquids, n.o.s. (Cyclohexane, n-Heptane, o-Xylene)
- **IMDG** FLAMMABLE LIQUID, N.O.S. (Cyclohexane, n-Heptane, o-Xylene, 1-methylnaphthalene), MARINE POLLUTANT
- **IATA** FLAMMABLE LIQUID, N.O.S. (Cyclohexane, n-Heptane, o-Xylene)

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· **Transport hazard class(es)**

· **DOT**



· **Class** 3 Flammable liquids
 · **Label** 3

· **IMDG**



· **Class** 3 Flammable liquids
 · **Label** 3

· **IATA**



· **Class** 3 Flammable liquids
 · **Label** 3

· **Packing group**
 · **DOT, IMDG, IATA** II

· **Environmental hazards:** Product contains environmentally hazardous substances:
 Cyclohexane

· **Marine pollutant:** Symbol (fish and tree)

· **Special precautions for user** Warning: Flammable liquids

· **Hazard identification number (Kemler code):** 33

· **EMS Number:** F-E, S-E

· **Stowage Category** B

· **Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code** Not applicable.

· **Transport/Additional information:**

· **DOT**

· **Quantity limitations** On passenger aircraft/rail: 5 L
 On cargo aircraft only: 60 L

· **IMDG**

· **Limited quantities (LQ)** 1L

· **Excepted quantities (EQ)** Code: E2
 Maximum net quantity per inner packaging: 30 ml
 Maximum net quantity per outer packaging: 500 ml

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· **UN "Model Regulation":** UN 1993 FLAMMABLE LIQUID, N.O.S. (CYCLOHEXANE, N-HEPTANE, O-XYLENE), 3, II

15 Regulatory information

· **Safety, health and environmental regulations/legislation specific for the substance or mixture**
No further relevant information available.

· **Sara**

· **Section 355 (extremely hazardous substances):**

None of the ingredients is listed.

· **Section 313 (Specific toxic chemical listings):**

CAS: 110-82-7 Cyclohexane

CAS: 95-47-6 o-Xylene

Phenanthrene, 98%

· **TSCA (Toxic Substances Control Act):**

Cyclohexane

ACTIVE

o-Xylene

ACTIVE

n-Heptane

ACTIVE

1-methylnaphthalene

ACTIVE

Phenanthrene, 98%

ACTIVE

· **Hazardous Air Pollutants**

CAS: 95-47-6 o-Xylene

Phenanthrene, 98%

· **Proposition 65**

· **Chemicals known to cause cancer:**

None of the ingredients is listed.

· **Chemicals known to cause reproductive toxicity for females:**

None of the ingredients is listed.

· **Chemicals known to cause reproductive toxicity for males:**

None of the ingredients is listed.

· **Chemicals known to cause developmental toxicity:**

None of the ingredients is listed.

· **Carcinogenic categories**

· **EPA (Environmental Protection Agency)**

CAS: 110-82-7 Cyclohexane

I

CAS: 95-47-6 o-Xylene

I

CAS: 142-82-5 n-Heptane

D

Phenanthrene, 98%

D

· **TLV (Threshold Limit Value)**

CAS: 95-47-6 o-Xylene

A4

CAS: 90-12-0 1-methylnaphthalene

A4

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· **NIOSH-Ca (National Institute for Occupational Safety and Health)**

None of the ingredients is listed.

· **GHS label elements** The product is classified and labeled according to the Globally Harmonized System (GHS).

· **Hazard pictograms**



GHS02 GHS07 GHS08

· **Signal word** *Danger*

· **Hazard-determining components of labeling:**

Cyclohexane

n-Heptane

· **Hazard statements**

Highly flammable liquid and vapor.

Causes skin irritation.

May cause drowsiness or dizziness.

May be fatal if swallowed and enters airways.

· **Precautionary statements**

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

Ground/bond container and receiving equipment.

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

Use only non-sparking tools.

Take precautionary measures against static discharge.

Avoid breathing dust/fume/gas/mist/vapors/spray

Wash thoroughly after handling.

Use only outdoors or in a well-ventilated area.

Wear protective gloves/protective clothing/eye protection/face protection.

If swallowed: Immediately call a poison center/doctor.

Specific treatment (see on this label).

Do NOT induce vomiting.

If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.

IF INHALED: Remove person to fresh air and keep comfortable for breathing.

Call a poison center/doctor if you feel unwell.

Take off contaminated clothing and wash it before reuse.

If skin irritation occurs: Get medical advice/attention.

In case of fire: Use CO2, powder or water spray to extinguish.

Store in a well-ventilated place. Keep container tightly closed.

Store in a well-ventilated place. Keep cool.

Store locked up.

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

· **Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

*

16 Other information

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

· **Department issuing SDS:** Environment protection department.

· **Contact:**

Date of Preparation / Last Revision:

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· **Date of preparation / last revision**

Revision 1.2, 06/05/2024: Reviewed SDS for accuracy. MH/STN

Revision 0.0, 05-29-2024: Creation date for SDS. STN

06/07/2024

· **Abbreviations and acronyms:**

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

EINECS: European Inventory of Existing Commercial Chemical Substances

ELINCS: European List of Notified Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

NFPA: National Fire Protection Association (USA)

HMIS: Hazardous Materials Identification System (USA)

VOC: Volatile Organic Compounds (USA, EU)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

PBT: Persistent, Bioaccumulative and Toxic

vPvB: very Persistent and very Bioaccumulative

NIOSH: National Institute for Occupational Safety

OSHA: Occupational Safety & Health

TLV: Threshold Limit Value

PEL: Permissible Exposure Limit

REL: Recommended Exposure Limit

BEI: Biological Exposure Limit

Flammable Liquids 2: Flammable liquids – Category 2

Skin Irritation 2: Skin corrosion/irritation – Category 2

Specific Target Organ Toxicity - Single Exposure 3: Specific target organ toxicity (single exposure) – Category 3

Aspiration Hazard 1: Aspiration hazard – Category 1

· *** Data compared to the previous version altered.**

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