

Safety Data Sheet

acc. to OSHA HCS

Printing date 06/07/2024

Reviewed on 06/07/2024

1 Identification

- **Product identifier**
- **Trade name:** ASTM D6591 Modified Cal Std
Method Aromatics by HPLC - C
- **Article number:** HOU067
- **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:**
n-Heptane
Cyclohexane

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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
 Fire = 3
 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: 142-82-5	<i>n</i> -Heptane	70.382%
CAS: 95-47-6	<i>o</i> -Xylene	13.905%
CAS: 110-82-7	Cyclohexane	13.905%
CAS: 90-12-0	1-methylnaphthalene	1.391%
	Phenanthrene, 98%	0.417%

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: 142-82-5	<i>n</i> -Heptane	500 ppm
CAS: 110-82-7	Cyclohexane	300 ppm
CAS: 90-12-0	1-methylnaphthalene	20 mg/m ³
	Phenanthrene, 98%	5.4 mg/m ³

· PAC-2:

CAS: 142-82-5	<i>n</i> -Heptane	830 ppm
CAS: 110-82-7	Cyclohexane	1700* ppm
CAS: 90-12-0	1-methylnaphthalene	61 mg/m ³
	Phenanthrene, 98%	59 mg/m ³

· PAC-3:

CAS: 142-82-5	<i>n</i> -Heptane	5000* ppm
CAS: 110-82-7	Cyclohexane	10000** 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: 142-82-5 *n*-Heptane

PEL Long-term value: 2000 mg/m³, 500 ppm

REL Long-term value: 350 mg/m³, 85 ppm
 Ceiling limit value: 1800* mg/m³, 440* ppm
 *15-min

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TLV	Short-term value: 500 ppm Long-term value: 400 ppm
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: 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
CAS: 90-12-0 1-methylnaphthalene	
TLV	Long-term value: 0.05 ppm SL 3 mg/100 cm ² , Skin, A4
Phenanthrene, 98%	
TWA	Short-term value: 0.2 mg/m ³
· Ingredients with biological limit values:	
CAS: 95-47-6 o-Xylene	
BEI	1.5 g/g creatinine LD50 Intraperitoneal: urine Time: end of shift LD50: Methylhippuric acids
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)

· **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

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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

· **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:	Gasoline-like
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):** 0.72762 g/cm³ (6.07199 lbs/gal)

· **Relative density** Not determined.

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- | | |
|---|--|
| · Vapor 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: | 98.2 % |
| VOC content: | 98.19 % |
| | 714.5 g/l / 5.96 lb/gal |
| Solids content: | 0.4 % |
| · 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)

Oral	LD50	132,327 mg/kg (rat)
Dermal	LD50	7,911 mg/kg
Inhalative	LC50/4h	79.1 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

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Phenanthrene, 98%	3
· NTP (National Toxicology Program)	
Phenanthrene, 98%	R
· 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. (n-Heptane, Cyclohexane, o-Xylene)
- **IMDG** FLAMMABLE LIQUID, N.O.S. (n-Heptane, Cyclohexane, o-Xylene, 1-methylnaphthalene), MARINE POLLUTANT
- **IATA** FLAMMABLE LIQUID, N.O.S. (n-Heptane, Cyclohexane, o-Xylene)

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Trade name: **ASTM D6591 Modified Cal Std**
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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: *n*-Heptane

· **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. (N-HEPTANE, CYCLOHEXANE, 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: 95-47-6 o-Xylene

CAS: 110-82-7 Cyclohexane

Phenanthrene, 98%

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

n-Heptane

ACTIVE

o-Xylene

ACTIVE

Cyclohexane

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: 142-82-5 n-Heptane

D

CAS: 95-47-6 o-Xylene

I

CAS: 110-82-7 Cyclohexane

I

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:**

n-Heptane

Cyclohexane

· **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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