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 - B

· Article number: HOU066

· Details of the supplier of the safety data sheet

· Manufacturer/Supplier: Aqua Solutions, Inc. 6913 Highway 225 DEER PARK, TX 77536 USA800-256-2586

· 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.



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

(Contd. on page 2)

Printing date 06/07/2024 Reviewed on 06/07/2024

Trade name: ASTM D6591 Modified Cal Std. Method Aromatics by HPLC - B

(Contd. of page 1)

· 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

- · Other hazards
- · Results of PBT and vPvB assessment
- · **PBT**: Not applicable.
- $\cdot vPvB$:

Phenanthrene, 98%

3 Composition/information on ingredients

- · Chemical characterization: Mixtures
- · Description: Mixture of the substances listed below with nonhazardous additions.

(Contd. on page 3)

Printing date 06/07/2024 Reviewed on 06/07/2024

Trade name: ASTM D6591 Modified Cal Std. Method Aromatics by HPLC - B

(Contd. of page 2)

D	*	itai or page 2)
· Dangerous components:		
CAS: 142-82-5	<u> </u>	49.359%
CAS: 110-82-7	Cyclohexane	26.724%
CAS: 95-47-6	o-Xylene	20.043%
CAS: 90-12-0	1-methylnaphthalene	3.341%
	Phenanthrene, 98%	0.535%

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.

(Contd. on page 4)

Printing date 06/07/2024 Reviewed on 06/07/2024

Trade name: ASTM D6591 Modified Cal Std. Method Aromatics by HPLC - B

Protective Action	on Criteria for Chemicals	(Contd. of page 3
<i>PAC-1:</i>	· · · · · · · · · · · · · · · · · · ·	
CAS: 142-82-5	n-Heptane	500 ppm
CAS: 110-82-7	Cyclohexane	300 ppm
CAS: 90-12-0	1-methylnaphthalene	20 mg/m³
	Phenanthrene, 98%	5.4 mg/m
PAC-2:		
CAS: 142-82-5	n-Heptane	830 ppm
CAS: 110-82-7	Cyclohexane	1700* ppm
CAS: 90-12-0	1-methylnaphthalene	61 mg/m³
	Phenanthrene, 98%	59 mg/m³
PAC-3:		
CAS: 142-82-5	n-Heptane	5000* ppm
CAS: 110-82-7	Cyclohexane	10000** ppm
CAS: 90-12-0	1-methylnaphthalene	360 mg/m^3

7 Handling and storage

- · Handling:
- · Precautions for safe handling

Ensure good ventilation/exhaustion at the workplace.

Phenanthrene, 98%

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			
	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		

(Contd. on page 5)

 $360 \, mg/m^3$

Printing date 06/07/2024 Reviewed on 06/07/2024

Trade name: ASTM D6591 Modified Cal Std. Method Aromatics by HPLC - B

	(Contd. of page 4)
TLV	Short-term value: 500 ppm
	Long-term value: 400 ppm
CAS:	110-82-7 Cyclohexane
PEL	Long-term value: 1050 mg/m³, 300 ppm
REL	Long-term value: 1050 mg/m³, 300 ppm
TLV	Long-term value: 100 ppm BEI
CAS:	95-47-6 o-Xylene
PEL	Long-term value: 435 mg/m³, 100 ppm
REL	Short-term value: 655 mg/m³, 150 ppm Long-term value: 435 mg/m³, 100 ppm
TLV	Long-term value: 20 ppm BEI, A4
CAS:	90-12-0 1-methylnaphthalene
TLV	Long-term value: 0.05 ppm SL 3 mg/100 cm2, Skin, A4
Phen	anthrene, 98%
TWA	Short-term value: 0.2 mg/m³
· Ingre	edients 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)
CAS:	95-47-6 o-Xylene
	1.5 g/g creatinine
	LD50 Intraperitoneal: urine
	Time: end of shift
	LD50: Methylhippuric acids

- · 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:



(Contd. on page 6)

Printing date 06/07/2024 Reviewed on 06/07/2024

Trade name: ASTM D6591 Modified Cal Std. Method Aromatics by HPLC - B

(Contd. of page 5)

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):	0.75948 g/cm³ (6.33786 lbs/gal)	
Relative density	Not determined.	

(Contd. on page 7)

Printing date 06/07/2024 Reviewed on 06/07/2024

Trade name: ASTM D6591 Modified Cal Std. Method Aromatics by HPLC - B

		(Contd. of page	
Vapor density	Not determined.		
Evaporation rate	Not determined.	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:	96.1 %		
VOC content:	96.13 %		
	730.1 g/l / 6.09 lb/gal		
Solids content:	0.5 %		
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:

· <i>LD/LC50</i> 1	· LD/LC50 values that are relevant for classification:			
ATE (Acute Toxicity Estimate)				
Oral	LD50	55,082 mg/kg (rat)		
Dermal	LD50	5,488 mg/kg		
Inhalative	LC50/4h	54.9 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

(Contd. on page 8)

Reviewed on 06/07/2024 Printing date 06/07/2024

Trade name: ASTM D6591 Modified Cal Std. Method Aromatics by HPLC - B

Phenanthrene, 98%	(Contd. of page 7)
· 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.

· 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)

Reviewed on 06/07/2024 Printing date 06/07/2024

Trade name: ASTM D6591 Modified Cal Std. Method Aromatics by HPLC - B

(Contd. of page 8) · Transport hazard class(es) $\cdot DOT$ · Class 3 Flammable liquids · Label · IMDG · Class 3 Flammable liquids · Label \cdot 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) Warning: Flammable liquids · Special precautions for user · Hazard identification number (Kemler code): 33 · EMS Number: *F-E*,<u>*S-E*</u> · Stowage Category · Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code Not applicable. · Transport/Additional information: $\cdot DOT$ · Quantity limitations On passenger aircraft/rail: 5 L On cargo aircraft only: 60 L · IMDG · Limited quantities (LQ) 1LCode: E2 · Excepted quantities (EQ) Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 500 ml (Contd. on page 10)

Printing date 06/07/2024 Reviewed on 06/07/2024

Trade name: ASTM D6591 Modified Cal Std. Method Aromatics by HPLC - B

(Contd. of page 9)

· 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 su	bstances):
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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):

n-Heptane	ACTIVE
Cyclohexane	ACTIVE
o-Xylene	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: 110-82-7	Cyclohexane	I	
CAS: 95-47-6	o-Xylene	I	
	Phenanthrene, 98%	D	

$\cdot TLV$	(Threshold	Limit	Value)
-------------	------------	-------	-------	---

. ,		
CAS: 95-47-6 o	-Xylene	A4
CAS: 90-12-0 1	-methylnaphthalene	A4

(Contd. on page 11)

Printing date 06/07/2024 Reviewed on 06/07/2024

Trade name: ASTM D6591 Modified Cal Std. Method Aromatics by HPLC - B

(Contd. of page 10)

· 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

- · 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:

(Contd. on page 12)

Printing date 06/07/2024 Reviewed on 06/07/2024

Trade name: ASTM D6591 Modified Cal Std. Method Aromatics by HPLC - B

(Contd. of page 11)

· 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.

US