

# Safety Data Sheet

acc. to OSHA HCS

Printing date 08/12/2024

Reviewed on 08/12/2024

## 1 Identification

- **Product identifier**
- **Trade name:** MECN:IPAC:Heptane 1:6:7 v/v Solution
- **Article number:** CHA050
- **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](mailto: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.

Eye Irritation 2A

H319 Causes serious eye 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  
Isopropyl Acetate

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· **Hazard statements**

Highly flammable liquid and vapor.  
 Causes skin irritation.  
 Causes serious eye 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.  
 If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.  
 Continue rinsing.  
 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.  
 If eye irritation persists: Get medical advice/attention.  
 In case of fire: Use CO<sub>2</sub>, 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 = 2  
 Fire = 4  
 Reactivity = 0

· **HMIS-ratings (scale 0 - 4)**



Health = 2  
 Fire = 4  
 Reactivity = 0

· **Other hazards**

· **Results of PBT and vPvB assessment**

· **PBT:** Not applicable.  
 · **vPvB:** Not applicable.

## 3 Composition/information on ingredients

· **Chemical characterization: Mixtures**

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

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· <b>Dangerous components:</b>		
CAS: 108-21-4	Isopropyl Acetate	48.56%
CAS: 142-82-5	n-Heptane	44.18%
CAS: 75-05-8	Acetonitrile, Reagent ACS Grade	7.26%

## 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. If symptoms persist, consult a doctor.
- **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:**  
CO<sub>2</sub>, 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.
- **Protective Action Criteria for Chemicals**

· <b>PAC-1:</b>		
CAS: 108-21-4	Isopropyl Acetate	200 ppm
CAS: 142-82-5	n-Heptane	500 ppm

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CAS: 75-05-8	Acetonitrile, Reagent ACS Grade	13 ppm
<b>· PAC-2:</b>		
CAS: 108-21-4	Isopropyl Acetate	2700* ppm
CAS: 142-82-5	n-Heptane	830 ppm
CAS: 75-05-8	Acetonitrile, Reagent ACS Grade	50 ppm
<b>· PAC-3:</b>		
CAS: 108-21-4	Isopropyl Acetate	16000** ppm
CAS: 142-82-5	n-Heptane	5000* ppm
CAS: 75-05-8	Acetonitrile, Reagent ACS Grade	150 ppm

## 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:**

<b>CAS: 108-21-4 Isopropyl Acetate</b>	
PEL	Long-term value: 950 mg/m <sup>3</sup> , 250 ppm
TLV	Short-term value: 150 ppm Long-term value: 100 ppm
<b>CAS: 142-82-5 n-Heptane</b>	
PEL	Long-term value: 2000 mg/m <sup>3</sup> , 500 ppm
REL	Long-term value: 350 mg/m <sup>3</sup> , 85 ppm Ceiling limit value: 1800* mg/m <sup>3</sup> , 440* ppm *15-min
TLV	Short-term value: 500 ppm Long-term value: 400 ppm
<b>CAS: 75-05-8 Acetonitrile, Reagent ACS Grade</b>	
PEL	Long-term value: 70 mg/m <sup>3</sup> , 40 ppm

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REL Long-term value: 34 mg/m<sup>3</sup>, 20 ppm

TLV Long-term value: 20 ppm  
Skin, A4

· **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 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

· **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:** Organic

· **Odor threshold:** Not determined.

· **pH-value:** Not determined.

· **Change in condition**

Melting point/Melting range: Undetermined.

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<b>Boiling point/Boiling range:</b>	36 °C (96.8 °F)
· <b>Flash point:</b>	-4 °C (24.8 °F)
· <b>Flammability (solid, gaseous):</b>	Highly flammable.
· <b>Auto igniting:</b>	215 °C (419 °F)
· <b>Decomposition temperature:</b>	Not determined.
· <b>Ignition temperature:</b>	Product is not selfigniting.
· <b>Danger of explosion:</b>	Product is not explosive. However, formation of explosive air/vapor mixtures are possible.
· <b>Explosion limits:</b>	
<b>Lower:</b>	1.1 Vol %
<b>Upper:</b>	8 Vol %
· <b>Vapor pressure at 20 °C (68 °F):</b>	61 hPa (45.8 mm Hg)
· <b>Vapor pressure at 50 °C (122 °F):</b>	190 hPa (142.5 mm Hg)
· <b>Density at 20 °C (68 °F):</b>	0.8 g/cm <sup>3</sup> (6.676 lbs/gal)
· <b>Relative density</b>	Not determined.
· <b>Vapor density</b>	Not determined.
· <b>Evaporation rate</b>	Not determined.
· <b>Solubility in / Miscibility with Water:</b>	Not miscible or difficult to mix.
· <b>Partition coefficient (n-octanol/water):</b>	Not determined.
· <b>Viscosity:</b>	
<b>Dynamic:</b>	Not determined.
<b>Kinematic:</b>	Not determined.
· <b>Solvent content:</b>	
<b>Organic solvents:</b>	92.7 %
<b>VOC content:</b>	92.74 %
	741.9 g/l / 6.19 lb/gal
<b>Solids content:</b>	0.0 %
· <b>Other information</b>	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.

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## 11 Toxicological information

- **Information on toxicological effects**

- **Acute toxicity:**

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

**ATE (Acute Toxicity Estimate)**

Oral	LD50	6,887 mg/kg
Dermal	LD50	15,152 mg/kg
Inhalative	LC50/4h	152 mg/l

- **Primary irritant effect:**

- **on the skin:** Irritant to skin and mucous membranes.

- **on the eye:** 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)**

None of the ingredients is listed.

- **NTP (National Toxicology Program)**

None of the ingredients is listed.

- **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:** Not applicable.

- **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.

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- **Uncleaned packagings:**
- **Recommendation:** Disposal must be made according to official regulations.

## 14 Transport information

<ul style="list-style-type: none"> <li>· <b>UN-Number</b></li> <li>· <b>DOT, IMDG, IATA</b></li> </ul>	UNI993
<ul style="list-style-type: none"> <li>· <b>UN proper shipping name</b></li> <li>· <b>DOT</b></li> <li>· <b>IMDG</b></li> <li>· <b>IATA</b></li> </ul>	<p><i>Flammable liquids, n.o.s. (n-Heptane, Isopropyl Acetate, acetonitrile)</i></p> <p><i>FLAMMABLE LIQUID, N.O.S. (n-Heptane, Isopropyl Acetate, acetonitrile), MARINE POLLUTANT</i></p> <p><i>FLAMMABLE LIQUID, N.O.S. (n-Heptane, Isopropyl Acetate, acetonitrile)</i></p>
<ul style="list-style-type: none"> <li>· <b>Transport hazard class(es)</b></li> <li>· <b>DOT</b></li> </ul>	<div style="text-align: center;">  </div> <p>3 Flammable liquids</p>
<ul style="list-style-type: none"> <li>· <b>Class</b></li> <li>· <b>Label</b></li> </ul>	3
<ul style="list-style-type: none"> <li>· <b>IMDG</b></li> </ul>	<div style="text-align: center;">  </div>
<ul style="list-style-type: none"> <li>· <b>Class</b></li> <li>· <b>Label</b></li> </ul>	3 Flammable liquids
<ul style="list-style-type: none"> <li>· <b>Label</b></li> </ul>	3
<ul style="list-style-type: none"> <li>· <b>IATA</b></li> </ul>	<div style="text-align: center;">  </div>
<ul style="list-style-type: none"> <li>· <b>Class</b></li> <li>· <b>Label</b></li> </ul>	3 Flammable liquids
<ul style="list-style-type: none"> <li>· <b>Label</b></li> </ul>	3
<ul style="list-style-type: none"> <li>· <b>Packing group</b></li> <li>· <b>DOT, IMDG, IATA</b></li> </ul>	II
<ul style="list-style-type: none"> <li>· <b>Environmental hazards:</b></li> <li>· <b>Marine pollutant:</b></li> </ul>	<p><i>Product contains environmentally hazardous substances: n-Heptane</i></p> <p><i>Symbol (fish and tree)</i></p>
<ul style="list-style-type: none"> <li>· <b>Special precautions for user</b></li> <li>· <b>Hazard identification number (Kemler code):</b></li> <li>· <b>EMS Number:</b></li> <li>· <b>Stowage Category</b></li> </ul>	<p><i>Warning: Flammable liquids</i></p> <p>33</p> <p>F-E,S-D</p> <p>B</p>

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· <b>Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code</b>	Not applicable.
· <b>Transport/Additional information:</b>	
· <b>DOT</b>	
· <b>Quantity limitations</b>	On passenger aircraft/rail: 5 L On cargo aircraft only: 60 L
· <b>IMDG</b>	
· <b>Limited quantities (LQ)</b>	5L
· <b>Excepted quantities (EQ)</b>	Code: E2 Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 500 ml
· <b>UN "Model Regulation":</b>	UN 1993 FLAMMABLE LIQUID, N.O.S. (N-HEPTANE, ISOPROPYL ACETATE, ACETONITRILE), 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: 75-05-8 | Acetonitrile, Reagent ACS Grade

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

Isopropyl Acetate	ACTIVE
n-Heptane	ACTIVE
Acetonitrile, Reagent ACS Grade	ACTIVE

· **Hazardous Air Pollutants**

CAS: 75-05-8 | Acetonitrile, Reagent ACS Grade

· **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: 75-05-8   Acetonitrile, Reagent ACS Grade	CBD, D

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· **TLV (Threshold Limit Value)**

CAS: 75-05-8 | Acetonitrile, Reagent ACS Grade

A4

· **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*

*Isopropyl Acetate*

· **Hazard statements**

*Highly flammable liquid and vapor.*

*Causes skin irritation.*

*Causes serious eye 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.*

*If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.*

*Continue rinsing.*

*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.*

*If eye irritation persists: Get medical advice/attention.*

*In case of fire: Use CO<sub>2</sub>, 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.*

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## 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:*

· **Date of preparation / last revision**

*Revision 1.2, 08-12-2024: Reviewed SDS for accuracy. STN/GW  
08/12/2024 / 1.1*

· **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*

*Flammable Liquids 2: Flammable liquids – Category 2*

*Skin Irritation 2: Skin corrosion/irritation – Category 2*

*Eye Irritation 2A: Serious eye damage/eye irritation – Category 2A*

*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