

Creation Date 04-Jul-2014

Revision Date 15-Oct-2015

Revision Number 2

## SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

### 1.1. Product identification

Product Description: **5-Methylhexanoic acid**  
 Cat No. : **457410000, 457410050, 457410250, 457411000**  
 CAS-No **628-46-6**  
 Molecular Formula **C7 H14 O2**

### 1.2. Relevant identified uses of the substance or mixture and uses advised against

Recommended Use Laboratory chemicals.  
 Uses advised against No Information available

### 1.3. Details of the supplier of the safety data sheet

Company Acros Organics BVBA  
 Janssen Pharmaceuticaaan 3a  
 2440 Geel, Belgium  
 E-mail address [begel.sdsdesk@thermofisher.com](mailto:begel.sdsdesk@thermofisher.com)

### 1.4. Emergency telephone number

For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11  
 Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No.**US**:001-800-424-9300 / **Europe**:001-703-527-3887

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

#### CLP Classification - Regulation (EC) No 1272/2008

#### Physical hazards

Substances/mixtures corrosive to metal

Category 1

#### Health hazards

Skin Corrosion/irritation

Category 1 C

Serious Eye Damage/Eye Irritation

Category 1

#### Environmental hazards

Based on available data, the classification criteria are not met

### 2.2. Label elements

# SAFETY DATA SHEET

5-Methylhexanoic acid

Revision Date 15-Oct-2015



**Signal Word**

**Danger**

## Hazard Statements

H290 - May be corrosive to metals  
H314 - Causes severe skin burns and eye damage

## Precautionary Statements

P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P310 - Immediately call a POISON CENTER or doctor/ physician  
P280 - Wear protective gloves/ protective clothing/ eye protection/ face protection  
P301 + P330 + P331 - IF SWALLOWED: Rinse mouth. Do NOT induce vomiting  
P303 + P361 + P353 - IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower  
P234 - Keep only in original container

## 2.3. Other hazards

No information available

## SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1. Substances

| Component                | CAS-No   | EC-No. | Weight % | CLP Classification - Regulation (EC) No 1272/2008                |
|--------------------------|----------|--------|----------|------------------------------------------------------------------|
| Hexanoic acid, 5-methyl- | 628-46-6 |        | >95      | Met. Corr. 1 (H290)<br>Skin Corr. 1C (H314)<br>Eye Dam. 1 (H318) |

Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

|                       |                                                                                                                                                                                                                                                             |
|-----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>General Advice</b> | Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.                                                                                                                                                           |
| <b>Eye Contact</b>    | Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required. Keep eye wide open while rinsing.                                                                                         |
| <b>Skin Contact</b>   | Wash off immediately with plenty of water for at least 15 minutes. Remove and wash contaminated clothing before re-use. Call a physician immediately.                                                                                                       |
| <b>Ingestion</b>      | Do not induce vomiting. Clean mouth with water. Never give anything by mouth to an unconscious person. Call a physician immediately.                                                                                                                        |
| <b>Inhalation</b>     | If breathing is difficult, give oxygen. Remove from exposure, lie down. Do not use mouth-to-mouth resuscitation if victim ingested or inhaled the substance; induce artificial respiration with a respiratory medical device. Call a physician immediately. |

# SAFETY DATA SHEET

5-Methylhexanoic acid

Revision Date 15-Oct-2015

**Protection of First-aiders** Use personal protective equipment.

## **4.2. Most important symptoms and effects, both acute and delayed**

None reasonably foreseeable. Causes burns by all exposure routes. . Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

## **4.3. Indication of any immediate medical attention and special treatment needed**

**Notes to Physician** Treat symptomatically.

## **SECTION 5: FIREFIGHTING MEASURES**

### **5.1. Extinguishing media**

#### **Suitable Extinguishing Media**

CO<sub>2</sub>, dry chemical, dry sand, alcohol-resistant foam.

#### **Extinguishing media which must not be used for safety reasons**

No information available.

### **5.2. Special hazards arising from the substance or mixture**

Thermal decomposition can lead to release of irritating gases and vapors. The product causes burns of eyes, skin and mucous membranes.

#### **Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Thermal decomposition can lead to release of irritating gases and vapors.

### **5.3. Advice for firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

## **SECTION 6: ACCIDENTAL RELEASE MEASURES**

### **6.1. Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Ensure adequate ventilation. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

### **6.2. Environmental precautions**

Should not be released into the environment. See Section 12 for additional ecological information.

### **6.3. Methods and material for containment and cleaning up**

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal.

### **6.4. Reference to other sections**

Refer to protective measures listed in Sections 8 and 13.

## **SECTION 7: HANDLING AND STORAGE**

### **7.1. Precautions for safe handling**

Wear personal protective equipment. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe vapors or spray mist. Do not ingest.

# SAFETY DATA SHEET

5-Methylhexanoic acid

Revision Date 15-Oct-2015

## 7.2. Conditions for safe storage, including any incompatibilities

Keep containers tightly closed in a dry, cool and well-ventilated place. Corrosives area. Do not store in metal containers.

## 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### Exposure limits

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

#### Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies.

#### Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents.

MDHS70 General methods for sampling airborne gases and vapours

MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

**Derived No Effect Level (DNEL)** No information available

| <u>Route of exposure</u>     | <u>Acute effects (local)</u> | <u>Acute effects (systemic)</u> | <u>Chronic effects (local)</u> | <u>Chronic effects (systemic)</u> |
|------------------------------|------------------------------|---------------------------------|--------------------------------|-----------------------------------|
| Oral<br>Dermal<br>Inhalation |                              |                                 |                                |                                   |

**Predicted No Effect Concentration (PNEC)** No information available.

### 8.2. Exposure controls

#### Engineering Measures

Ensure that eyewash stations and safety showers are close to the workstation location.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

#### Personal protective equipment

##### Eye Protection

Goggles (European standard - EN 166)

##### Hand Protection

Protective gloves

| <u>Glove material</u>            | <u>Breakthrough time</u>             | <u>Glove thickness</u> | <u>EU standard</u> | <u>Glove comments</u><br>(minimum requirement) |
|----------------------------------|--------------------------------------|------------------------|--------------------|------------------------------------------------|
| Natural rubber<br>Nitrile rubber | See manufacturers<br>recommendations |                        | EN 374             |                                                |

# SAFETY DATA SHEET

5-Methylhexanoic acid

Revision Date 15-Oct-2015

|              |   |
|--------------|---|
| Neoprene     | - |
| PVC          |   |
| Butyl rubber |   |

**Skin and body protection** Long sleeved clothing

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.

(Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

## Respiratory Protection

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.

To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

## Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

**Recommended Filter type:** Organic gases and vapours filter Type A Brown conforming to EN14387 Particulates filter conforming to EN 143 Acid gases filter Type E Yellow

## Small scale/Laboratory use

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

**Recommended half mask:-** Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

When RPE is used a face piece Fit Test should be conducted

## Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

## Environmental exposure controls

No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

### 9.1. Information on basic physical and chemical properties

|                                                |                          |                                          |
|------------------------------------------------|--------------------------|------------------------------------------|
| <b>Appearance</b>                              | Colorless Amber          |                                          |
| <b>Physical State</b>                          | Liquid                   |                                          |
| <b>Odor</b>                                    | No information available |                                          |
| <b>Odor Threshold</b>                          | No data available        |                                          |
| <b>pH</b>                                      | No information available |                                          |
| <b>Melting Point/Range</b>                     | No data available        |                                          |
| <b>Softening Point</b>                         | No data available        |                                          |
| <b>Boiling Point/Range</b>                     | 121 °C / 249.8 °F        | 30 mmHg                                  |
| <b>Flash Point</b>                             | > 102 °C / > 215.6 °F    | <b>Method -</b> No information available |
| <b>Evaporation Rate</b>                        | No data available        |                                          |
| <b>Flammability (solid,gas)</b>                | Not applicable           | Liquid                                   |
| <b>Explosion Limits</b>                        | No data available        |                                          |
| <b>Vapor Pressure</b>                          | No data available        |                                          |
| <b>Vapor Density</b>                           | No data available        | (Air = 1.0)                              |
| <b>Specific Gravity / Density</b>              | 0.905                    |                                          |
| <b>Bulk Density</b>                            | Not applicable           | Liquid                                   |
| <b>Water Solubility</b>                        | Slightly soluble         |                                          |
| <b>Solubility in other solvents</b>            | No information available |                                          |
| <b>Partition Coefficient (n-octanol/water)</b> |                          |                                          |
| <b>Autoignition Temperature</b>                | No data available        |                                          |
| <b>Decomposition Temperature</b>               | No data available        |                                          |
| <b>Viscosity</b>                               | No data available        |                                          |
| <b>Explosive Properties</b>                    | No information available |                                          |
| <b>Oxidizing Properties</b>                    | No information available |                                          |

# SAFETY DATA SHEET

5-Methylhexanoic acid

Revision Date 15-Oct-2015

## 9.2. Other information

Molecular Formula C7 H14 O2  
Molecular Weight 130.18

## SECTION 10: STABILITY AND REACTIVITY

### 10.1. Reactivity

None known, based on information available

### 10.2. Chemical stability

Stable under recommended storage conditions

### 10.3. Possibility of hazardous reactions

Hazardous Polymerization Hazardous polymerization does not occur.  
Hazardous Reactions None under normal processing.

### 10.4. Conditions to avoid

Incompatible products. Excess heat.

### 10.5. Incompatible materials

Bases. Oxidizing agents. . Metals.

### 10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Thermal decomposition can lead to release of irritating gases and vapors.

## SECTION 11: TOXICOLOGICAL INFORMATION

### 11.1. Information on toxicological effects

#### Product Information

#### (a) acute toxicity;

|            |                   |
|------------|-------------------|
| Oral       | No data available |
| Dermal     | No data available |
| Inhalation | No data available |

(b) skin corrosion/irritation; Category 1 C

(c) serious eye damage/irritation; Category 1

#### (d) respiratory or skin sensitization;

|             |                   |
|-------------|-------------------|
| Respiratory | No data available |
| Skin        | No data available |

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

# SAFETY DATA SHEET

5-Methylhexanoic acid

Revision Date 15-Oct-2015

|                                            |                                                                                                                                                                                                                                                            |
|--------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Target Organs                              | No information available.                                                                                                                                                                                                                                  |
| (j) aspiration hazard;                     | No data available                                                                                                                                                                                                                                          |
| Other Adverse Effects                      | The toxicological properties have not been fully investigated. See actual entry in RTECS for complete information                                                                                                                                          |
| Symptoms / effects, both acute and delayed | Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation |

## SECTION 12: ECOLOGICAL INFORMATION

|                                                                                                                                    |                                                                                                                                                                                                                                                                                                                            |
|------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>12.1. Toxicity</b><br>Ecotoxicity effects                                                                                       | Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.                                                                                                                                                                                                |
| <b>12.2. Persistence and degradability</b><br>Persistence                                                                          | May persist, based on information available.                                                                                                                                                                                                                                                                               |
| <b>12.3. Bioaccumulative potential</b>                                                                                             | May have some potential to bioaccumulate                                                                                                                                                                                                                                                                                   |
| <b>12.4. Mobility in soil</b>                                                                                                      | Spillage unlikely to penetrate soil The product is insoluble and floats on water The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces Is not likely mobile in the environment due its low water solubility. Will likely be mobile in the environment due to its volatility. |
| <b>12.5. Results of PBT and vPvB assessment</b>                                                                                    | No data available for assessment.                                                                                                                                                                                                                                                                                          |
| <b>12.6. Other adverse effects</b><br>Endocrine Disruptor Information<br>Persistent Organic Pollutant<br>Ozone Depletion Potential | This product does not contain any known or suspected endocrine disruptors<br>This product does not contain any known or suspected substance<br>This product does not contain any known or suspected substance                                                                                                              |

## SECTION 13: DISPOSAL CONSIDERATIONS

|                                       |                                                                                                                                                                                                                            |
|---------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>13.1. Waste treatment methods</b>  |                                                                                                                                                                                                                            |
| Waste from Residues / Unused Products | Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.                                                     |
| Contaminated Packaging                | Dispose of this container to hazardous or special waste collection point.                                                                                                                                                  |
| European Waste Catalogue (EWC)        | According to the European Waste Catalogue, Waste Codes are not product specific, but application specific.                                                                                                                 |
| Other Information                     | Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains. Do not dispose of waste into sewer. Large amounts will affect pH and harm aquatic organisms. |

## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

|                                         |                                          |
|-----------------------------------------|------------------------------------------|
| <b>14.1. UN number</b>                  | UN3265                                   |
| <b>14.2. UN proper shipping name</b>    | CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S |
| <b>14.3. Transport hazard class(es)</b> | 8                                        |
| <b>14.4. Packing group</b>              | III                                      |

### ADR

ACR45741

# SAFETY DATA SHEET

5-Methylhexanoic acid

Revision Date 15-Oct-2015

**14.1. UN number** UN3265  
**14.2. UN proper shipping name** CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S  
**14.3. Transport hazard class(es)** 8  
**14.4. Packing group** III

## IATA

**14.1. UN number** UN3265  
**14.2. UN proper shipping name** CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S  
**14.3. Transport hazard class(es)** 8  
**14.4. Packing group** III

**14.5. Environmental hazards** No hazards identified

**14.6. Special precautions for user** No special precautions required

**14.7. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code** Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

### 15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

**International Inventories** X = listed

| Component                | EINECS | ELINCS | NLP | TSCA | DSL | NDSL | PICCS | ENCS | IECSC | AICS | KECL |
|--------------------------|--------|--------|-----|------|-----|------|-------|------|-------|------|------|
| Hexanoic acid, 5-methyl- | -      | -      |     | X    | -   | X    | X     | X    | -     | X    | -    |

### National Regulations

Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment.  
Take note of Dir 94/33/EC on the protection of young people at work  
Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work

### 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

### Full Text of H-/EUH-Statements Referred to Under Section 3

H318 - Causes serious eye damage  
H290 - May be corrosive to metals  
H314 - Causes severe skin burns and eye damage

### Legend

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**TWA** - Time Weighted Average

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

**PNEC** - Predicted No Effect Concentration

**LD50** - Lethal Dose 50%



# SAFETY DATA SHEET

5-Methylhexanoic acid

Revision Date 15-Oct-2015

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - Volatile Organic Compounds

## Key literature references and sources for data

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

## Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

**Creation Date** 04-Jul-2014

**Revision Date** 15-Oct-2015

**Revision Summary** SDS sections updated, 2, 3, 10, 14, 16.

**This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006**

## Disclaimer

The information provided on this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other material or in any process, unless specified in the text.

**End of Safety Data Sheet**