Product Description and Handling Guide

Crotonaldehyde

2-Butenal
3-Methylacrolein
CAS no. 4170-30-3
EC no. 224-030-0

Product description

Crotonaldehyde, which is obtained by aldol condensation from acetaldehyde, is an almost colorless to pale yellow, highly flammable liquid with a lachrymatory effect and a pungent odor. It has poor solubility in water but is readily soluble in the usual organic solvents such as alcohols, ether and boiling point fractions of petroleum. In the presence of air, i.e. oxygen, Crotonaldehyde tends first to form a peroxide and then to oxidize to form crotonic acid, whereas in the presence of mineral acids (traces) it tends to polymerize and, in the presence of alkalis on heating, it also tends to condense or resinify.

Crotonaldehyde combines with water at normal pressure to form an azeotrope containing about 25% water boiling at 84 °C. Because of its aldehyde function and the conjugated olefinic double bond within the aldehyde, Crotonaldehyde can enter into numerous reactions and is therefore an important starting product for chemical synthesis. Crotonaldehyde acts as an effective solvent for numerous vegetable and mineral oils, fats, waxes, natural and synthetic resins as well as elementary sulphur.

Possible applications

One of the main applications is as a precursor of fine chemicals. Sorbic acid, a food preservative and trimethylhydroquinone, a precursor to the Vitamin E, are prepared from Crotonaldehyde.

Crotonaldehyde is used for the manufacture of crotonic acid and is employed as a comonomer and a flow-promoting agent for alkyd resins.

Crotyl alcohol, n-butanal and n-butanol are obtained by reduction of Crotonaldehyde. With alcohols Crotonaldehyde forms alkoxy butyraldehyde; for instance with methanol it forms 3-methoxy butanal and, after hydrogenation, 3-methoxy butanol. Like Butoxyl (3-methoxy-n-butyl acetate), it is suitable for use as a solvent.

Crotonylidene ureas, which are used as slow-release fertilizers, are obtained as a result of the reaction of Crotonaldehyde with urea. Crotonaldehyde is also used in the production of thiophenes, quinaldines, pyridines, pharmaceuticals, dyes and pesticides.
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Characteristic data

<table>
<thead>
<tr>
<th>Typical Properties</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molar mass</td>
<td>g/mol</td>
</tr>
<tr>
<td>Boiling point at 1013 hPa</td>
<td>°C</td>
</tr>
<tr>
<td>Melting temperature</td>
<td>°C</td>
</tr>
<tr>
<td>Density at 20 °C (DIN 51 757)</td>
<td>g/cm³</td>
</tr>
<tr>
<td>Refractive index n D at 10 °C (DIN 51 423)</td>
<td></td>
</tr>
<tr>
<td>Vapour pressure at 25 °C</td>
<td>hPa</td>
</tr>
<tr>
<td>Vapor density (Air=1)</td>
<td></td>
</tr>
<tr>
<td>Water Solubility at 20 °C</td>
<td>g/l</td>
</tr>
<tr>
<td>Water absorption at 20 °C</td>
<td>%(w/w)</td>
</tr>
</tbody>
</table>

These characteristic data are intended for the purpose of product description and are not the subject of continuous monitoring.

Further physical properties and characteristic data as well as information on safety and handling are listed in the material safety data sheet and the sales specifications. Please consult www.celanese.com

Shelf life

The shelf life of Crotonaldehyde is six months. Because of its marked tendency to oxidation and polymerization (discoloration), Crotonaldehyde must be blanketed with nitrogen during storage and further processing. Even so, the product has only limited storage stability.

The shelf life dates from the day of packaging, for bulk deliveries this is the day of loading. This period is in general applicable to material stored under conditions recommended by Celanese Chemicals.

Storage

<table>
<thead>
<tr>
<th>Recommended Blanketing</th>
<th>Dry Nitrogen¹²³</th>
</tr>
</thead>
<tbody>
<tr>
<td>Recommended Temperature range:</td>
<td></td>
</tr>
<tr>
<td>Maximum¹</td>
<td>100 °F (37.8 °C)</td>
</tr>
<tr>
<td>Minimum</td>
<td>0 °F (-17.8 °C)</td>
</tr>
<tr>
<td>Recommended pressure</td>
<td>Atmospheric</td>
</tr>
</tbody>
</table>

Bulk Quantities: Outside, detached tanks
Small Containers: Cool, dry, well ventilated area

Handling

- Thoroughly review Material Safety Data Sheet before handling product.
- Keep containers closed when not in use.
- Open containers slowly to allow any excess pressure to vent.
- Keep away from heat, sparks, flame or other sources of ignition.
- Protect small containers from physical damage.
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- Use proper electrical grounding and bonding procedures when loading, unloading and transferring.
- Refer to the Material Safety Data Sheet for more information on materials to avoid.
- Use spark-resistant tools.
- Electrical equipment and circuits in all storage and handling areas must conform to requirements of national electrical code (Articles 500 and 501) for hazardous location.
- Do not load into compartments adjacent to heated cargos.

1. Do not use air because explosive peroxides will form.
2. See the National Fire Protection Agency (NFPA) #30 “Flammable and Combustible Liquids Code” and consult with qualified fire protection specialists to determine specific storage tank design requirements.
3. Refer to NFPA #77 “Static Electricity” for proper electrical grounding procedures.
4. Elevated temperature and/or contamination may promote polymerization.

Crotonaldehyde is available from Celanese Chemicals as bulk material.

Materials for storage and transport

<table>
<thead>
<tr>
<th>Unit / element</th>
<th>Acceptable Material</th>
<th>Alternate Material</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tank</td>
<td>Stainless Steel¹</td>
<td></td>
</tr>
<tr>
<td>Piping</td>
<td>Stainless Steel¹</td>
<td>Carbon Steel³,⁴</td>
</tr>
<tr>
<td>Valves</td>
<td>Stainless Steel¹</td>
<td>Cast Iron, Carbon Steel³,⁴</td>
</tr>
<tr>
<td>Pumps</td>
<td>Stainless Steel¹</td>
<td>Cast Iron, Carbon Steel³,⁴</td>
</tr>
<tr>
<td>Relief Valves</td>
<td>Stainless Steel¹</td>
<td>Cast Iron, Carbon Steel³,⁴</td>
</tr>
<tr>
<td>Gaskets</td>
<td>Glass filled PTFE²</td>
<td></td>
</tr>
<tr>
<td>Pump Seals</td>
<td>Mechanical Seal: Double mechanical seal, back-to-back arrangement carbon to silicon carbide faces</td>
<td>Mechanical Seal: carbon to tungsten carbide faces, EPDM⁶ O-rings</td>
</tr>
<tr>
<td>Valve Packing</td>
<td>PTFE³</td>
<td>Graphite</td>
</tr>
<tr>
<td>Pipe End Connections</td>
<td>Welded and flanged system</td>
<td>Threaded with PTFE³ tape thread lubricant</td>
</tr>
<tr>
<td>Heat Exchanger</td>
<td>Product side: Stainless Steel¹</td>
<td></td>
</tr>
<tr>
<td>Hoses</td>
<td>Stainless Steel¹</td>
<td>EPDM⁶</td>
</tr>
<tr>
<td>Tank Car</td>
<td>Stainless Steel¹</td>
<td>Carbon Steel³,⁴</td>
</tr>
</tbody>
</table>

1. Type 304 or 316 Stainless Steel
2. Lining refers to high baked phenolic resin.
3. May be used if an increase of iron content, color or the presence of high boiling point impurities are not a problem.
4. Maximum storage temperature 120 °F (49 °C)
5. Polytetrafluoroethylene.

*For further information on safety and handling, please use the following link: [http://www.celanese.com/msds/](http://www.celanese.com/msds/)*

**Other Product Information:**

The following statements about Crotonaldehyde manufactured at Celanese are based to the best of our manufacturing and process knowledge. The practice of providing this information to customers is for their convenience. It does not alter the terms and conditions of sale, including any warranties or limitations on liability, applicable to the underlying commercial transaction involving the product to which this certification applies. We believe this information to be accurate and reliable, but customers should make their own determination on the suitability of this product for a particular application.

**Chemical Inventory Status**

The substance is listed in the following chemical inventories:

<table>
<thead>
<tr>
<th>Chemical Inventory Status</th>
<th>Listed</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>AICS (Australia)</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>DSL (Canada)</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>IECSC (China)</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>EINECS (Europe)</td>
<td>X</td>
<td>EC-No.: 224-030-0</td>
</tr>
<tr>
<td>ENCS (Japan)</td>
<td>X</td>
<td>Japanese ENCS Number (2)-524</td>
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<tr>
<td>ISHL (Japan)</td>
<td>X</td>
<td>Japanese ISHL Number (2)-524</td>
</tr>
<tr>
<td>KECI (Korea)</td>
<td>X</td>
<td>Korean ID Number: KE-05-0370 / 97-1-270</td>
</tr>
<tr>
<td>NZIoC (New Zealand)</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>PICCS (Philippines)</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>TSCA (USA)</td>
<td>X</td>
<td></td>
</tr>
</tbody>
</table>

**REACH**

REACH (“Registration, Evaluation, Authorization and Restriction of Chemicals”) Celanese is aware of the obligations imposed by the European Union legislation REACH on EU manufacturers and importers as well as on downstream users. We are obliged to comply with the requirements of the REACH legislation relating to our European manufacturing facilities, our own imports as well as our obligations as a downstream user in the European chemical industry. Should you require additional information, please contact Celanese at REACH@celanese.com
Animal Origin, Genetically Modified Organisms

**BSE/TSE Statement**
To the best of our knowledge Crotonaldehyde and the raw materials used in the production of this material are not derived from human or animal origin.

**Genetically Modified Organisms**
To the best of our knowledge this product is not based on raw materials obtained through genetically modified organisms. GMOs and biotechnical means are not used during the manufacturing process.

**Allergens Guide**
Celanese Acetyl Intermediates does not use any ingredients of animal or plant origin in the manufacture of Crotonaldehyde (CAS no. 4170-30-3). Therefore, we can certify that the supplied Crotonaldehyde does not contain any of the main food allergens (Peanut, Soya, Bean, Milk, Egg, Fish, Peas, Barley, Lupine, Mollusks). Crotonaldehyde is manufactured through an entirely synthetic process and will not contain any gluten. No nutritional data is available for Crotonaldehyde.

**Kosher**
Crotonaldehyde manufactured by Celanese is Kosher certified. Certificate is available on request.
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