From: David Egilman [degilman@neveragainconsulting.com]
Sent: Sunday, August 28, 2011 9:15 AM
To: David Egilman; NIOSH Docket Office (CDC)
Cc: hank@egilman.com; kxx2@cdc.gov; Degilman@egilman.com; hank@egilman.com
Subject: RE: 245 - Criteria for a Recommended Standard: Occupational Exposure to Diacetyl and 2,3-pentanedione

The attachments will be sent separately since your email system rejected them.

August 28, 2011

Dear Sir/Ms:

Attached is a peer reviewed paper on the diacetyl TLV. It comes to the same conclusion as does your criteria document (safe level is below 1 ppB). Also attached are the PFTs and exposure measurements for ConAgra QA workers who were followed for 8-12 months. The importance of these findings are noted in the peer reviewed paper attached. Lockey’s published paper asserted that none of the QA workers had obstructive lung abnormalities. [http://erj.ersjournals.com/content/34/1/63.full] As you can see this was not true. In addition NIOSH reported disease in QA workers in one of the ConAgra plants. These cases were excluded from Lockey’s study.

At the diacetyl hearing, I discussed Morgan’s study of 2,3 pentanedione which should be considered at least as peer reviewed as the MSDS sheets that NIOSH cites for key information on diacetyl and pentanedione. Poster Board 914. Lung Function and Pathogenesis of Bronchiolitis Obliterans in Rats Exposed to 2,3-Pentanedione D. L. Morgan; H. C. Price; C. L. Johnson; M. P. Jokinem; W. M. Gwinn; G. P. Flake [http://www.niehs.nih.gov/news/events/pastmg/2011/sot/sot2011.cfm]


Since the criteria document calls for ALARA (detection limit TLV) for pentanedione this should be explained more clearly. NIOSH proposes ZERO exposure and you should say so.

Finally Ezrailson published a letter (below) that indicated that due to its chemical structure diacetyl could be a carcinogen:

To the Editor:

Kreiss et al. (Aug. 1 issue) report a high incidence of bronchiolitis obliterans at a microwave-popcorn factory. The chemical diacetyl (2,3-butanedione) was singled out as a possible causal agent of this deadly condition and other medical problems found in workers in this plant. As a chemist, biochemist, and toxicologist, I would like to point out that 2,3-butanedione is in chemical equilibrium with 1,3-butane-diene-2,3-diol (Figure 1 Chemicals 2,3-Butanedione and 1,3-Butane-Diene-2,3-Diol, and Their Expected Product, 1,3-Butane-Diepoxide-2,3-Diol.). This phenomenon, which is well known in organic chemistry, is called ketoenol tautomerism. This isomer is expected to be very reactive with oxygen both at room temperature and on heating. Thus, 1,3-butane-diepoxide-2,3-diol would be expected as
a product. Although the parent compound is known to be reactive with arginine, the diepoxide is of particular interest, since butadiene diepoxide is a known human carcinogen. The appropriate government agencies must investigate and evaluate whether diacetyl should be banned from food products.

Edward G. Ezrailson, Ph.D.
2308 West Settler’s Way, The Woodlands, TX 77380
edez1@prodigy.net

Letters to NEJM are peer reviewed prior to publication by the editors and often by others and reviewed by the authors of the paper to which they refer.

Finally I attach BASF’s 1993 diacetyl toxicology study which is cited in many corporate MSDS sheets. This provides LC 50 data and pathologic evidence of lung disease in one rat. If NIOSH can cite MSD sheets as you do then NIOSH should be able to use this LC 50 data.

If you have any questions please do not hesitate to get in touch with me. I often can access information that companies are forced to produce in legal discovery but fail to report to the EPA under TOSCA. I believe BASF may have reported its study to the EPA. I know some companies did report health information to the EPA including Chemtura.

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Brown University
8 North Main Street
Attleboro, Massachusetts 02703
Cell 508-472-2809
Office 508-226-5091
Fax 425-699-7033
A Proposal for a Safe Exposure Level for Diacetyl

DAVID S. EGILMAN, JOHN HENRY SCHILLING, LELIA MENENDEZ

Diacetyl is a naturally occurring compound that has been used in concentrated form as a food additive, particularly in butter flavorings. Inhalation of diacetyl and butter flavoring fumes has caused a variety of respiratory diseases in workers and consumers including bronchiolitis obliterans (BO), a relatively rare, severe, and irreversible lung disease. A safe level of exposure to diacetyl has not been established. We review the literature on diacetyl and flavoring toxicity and critique a recent proposal for an occupational exposure limit (OEL) of 0.2 ppm for diacetyl. We present unpublished data and novel analyses in support of our proposal for a safe level of exposure. Our findings indicate that a safe level of exposure exists around or below a time-weighted average of 1 ppb for an eight-hour workday. The levels of exposure we found to be unsafe include ranges that popcorn consumers may potentially be exposed to, indicating a risk of severe lung disease (including BO) for some consumers. Key words: diacetyl, butter flavorings, popcorn lung, occupational exposure limit, bronchiolitis obliterans, safe exposure level, occupational disease

INT J OCCUP ENVIRON HEALTH 2011;17:122-134

Diacetyl (IUPAC systematic name: 2,3-butane-dione) is a vicinal diketone (two adjacent C=O groups) with the molecular formula C₄H₆O₂.¹ Diacetyl occurs naturally in a variety of foods including milk, milk products, and coffee, and is produced during the fermentation of alcoholic beverages.² It is used as a food additive because of the buttery flavor it imparts.² Prior to the advent of microwave popcorn, diacetyl levels in finished products were relatively low.³ Generally, exposure levels from these products were below the measurable threshold although often above the odor threshold of 1.5 ppb.⁴ The need to produce highly concentrated flavorings for microwave popcorn resulted in much higher diacetyl exposure levels in worker and consumer breathing zones, often in the range of 4–13 ppm.⁵

Inhalation of diacetyl and butter flavoring fumes has caused lung disease in workers, including bronchiolitis obliterans (BO), a relatively rare, severe, and irreversible lung disease.² As a result, hundreds of workers and some popcorn consumers have sued diacetyl, flavoring, and microwave popcorn manufacturers for compensation, resulting in hundreds of millions of dollars in verdicts.⁶

In response to this recent litigation, companies that use diacetyl in food manufacturing hired Toxicology Excellence for Risk Assessment (TERA) to develop a proposal for a "safe level" of diacetyl for use in defending lawsuits.

The current regulatory framework being proposed by California and Federal OSHA will likely be limited to establishing performance based exposure standards without establishing either an exposure limit or a threshold for safety for diacetyl. This will leave employees in the food processing industries confused regarding the safety of diacetyl as well as continue to expose companies who handle diacetyl to potential implied legal liability. [Emphasis added]⁷

TERA’S OCCUPATIONAL EXPOSURE LIMIT IS DERIVED FROM SELECT LIMITED DATA

The TERA researchers proposed an occupational exposure limit (OEL) of 0.2 ppm for a permissible exposure to diacetyl over the course of an eight-hour workday.⁸ TERA’s proposed OEL is based on a single animal experiment involving a total of 30 exposed mice and 10 controls, only 15 of which were exposed for up to 90 hours per week for 12 weeks.⁹ As a sponsor company, ConAgra was "asked to review the material and provide technical comment" (pg. 295). ConAgra did not provide TERA with confidential data they possess relating to diacetyl’s toxicity (Melissa Kohrman-Vincent, personal communication, 7/25/2010). This confidential data, which has been released pursuant to legal discovery includes the underlying data from an epidemiological study suggesting a health risk to popcorn consumers, and a quantitative structure activity relationship (QSAR) analysis, which found that diacetyl’s toxicity was comparable to isocyanates.¹⁰,¹¹ Isocyanates have a TLV of 1 ppb, 200 times lower than TERA’s proposed OEL for diacetyl.¹²

TERA Fails to Include Epidemiological Studies in their OEL Determination

As previously noted, TERA bases their OEL solely on the analysis of one mouse experiment from a single paper.⁹ The use of quality epidemiology studies in determining human exposure guidelines is well established. For example, a review of the use of animal studies to determine human risks states that "Threshold
Emissions from Cooking Microwave Popcorn

JACKY A. ROSATI and KENNETH A. KREBS
U.S. Environmental Protection Agency, National Risk Management Research Laboratory, RTP, NC 27711

XIAOYU LIU
U.S. Environmental Protection Agency, National Risk Management Research Laboratory, RTP, NC 27711; Arcadis G & M, RTP, NC 27711

This study characterized chemicals released into a chamber in the process of cooking microwave popcorn. Seventeen types of microwave popcorn from eight different brands were studied. The work proceeded in two phases: phase one investigated chemicals emitted during popping and opening, phase two investigated chemicals emitted at discrete intervals from 0–40 minutes post-pop opening. The research was performed using a microwave oven enclosed in a chamber with ports for air sampling of particulate matter (PM) and volatile organic compounds (VOCs). VOCs in the air samples were identified and quantified using gas chromatography/mass spectrometry (GC/MS). PM was characterized using both an aerodynamic particle sizer (APS) and a scanning mobility particle sizer (SMPS) to cover a full range of emitted sizes. The compounds measured during popping and opening included butter flavoring components such as diacetyl, butyric acid, acetoins, propylene glycol, 2-nonanone, and triacetin and bag components such as p-xylene and perfluorinated alcohol 8:2 telomer. The greatest chemical quantity is emitted when the bag is opened post-popping; more than 80% of the total chemical emissions occur at this time.

Keywords air sampling, diacetyl, perfluorinated compounds, volatiles

INTRODUCTION

This study identified and quantified chemical emissions released in the process of popping and opening a bag of microwave popcorn. Microwave popcorn, a product that is used extensively worldwide and in a large number of households and businesses in America, is thought to have a detrimental effect on lung health in the manufacturing industry (Kreiss et al., 2002; Kullman et al., 2005). This research was initiated in response to an occupational incident in 2000 in which eight workers at a microwave popcorn production plant in Missouri were diagnosed with the severe lung disease, bronchiolitis obliterans (Kreiss et al., 2002; Kullman et al., 2005). These plant workers were exposed to not only the raw corn and salt used in microwave popcorn production, but the oil, flavorings, and the microwaveable packagings (Kreiss et al., 2002; Kullman et al., 2005). The National Institute for Occupational Safety and Health (NIOSH) identified more than 100 volatile organic compounds inside of the Missouri plant (Kullman et al., 2005). Quality control (QC) personnel, who pop corn and open bags, had a high incidence of respiratory and dermal symptoms (Kanwal et al., 2006; Kreiss et al., 2002). NIOSH scientists confirm that workers in the QC areas have shown an increased risk of lung disease (Kanwal et al., 2006). This prompted EPA’s interest in what is released into the immediate environment when microwaving popcorn, and its potential to impact indoor air quality.

Seventeen types of microwave popcorn from eight different brands were studied. Data on volatile chemicals produced from microwave popcorn packaging during cooking were documented previously in 1993 (McNeal and Holllfield, 1993; Risch, 1993), but some manufacturers have changed their bag formulations. Limited data were available on the indoor concentrations of particulate matter less than 10 microns in diameter (PM_{10}) and particulate matter less than 2.5 microns in diameter (PM_{2.5}) released during the popping of a single type of microwave popcorn (Fortmann et al., 2001). No data on particulate matter (PM), characterization, flavoring, or corn emissions during the cooking of microwave popcorn, was found in the literature. Thus, this is the first study to take a comprehensive look at chemicals released while microwaving an entire conventional microwave popcorn product.
Safety data sheet
according to Regulation (EC) No 453/2010

Diacetyl

1. IDENTIFICATION OF THE SUBSTANCE AND OF THE COMPANY

1.1 Product identifier
Chemical name: 2,3-Butanedione
Synonyms: Butanedione, Butane-2,3-dione, 2,3-Butadiol, Macetyl, Dimethyl diketone,
2,3-Dimethyl glyoxal.
Formula: C₇H₈O₂
Molecular mass: 86.09
CAS-No.: 431-03-8
EC-No.: 207-069-8
Registration number:

1.2 Relevant identified uses of the substance and uses advised against
Flavoursing agent.

1.3 Details of the supplier of the safety data sheet
Manufacturer: Illovo Sugar (South Africa) Limited
Address: Gleneagles Park no. 3C
Mount Edgecombe
4300 South Africa
Telephone number: +27 31 508 43 00
Telefax number: +27 31 508 43 10
E-mail address: treed@illovo.co.za

Only representative: Otentic Customs BV
Address: Rederijweg 25, 4906 CX Oosterhout, The Netherlands
Telephone number: +31 162 48 80 65

1.4 Emergency telephone numbers
- Local South Africa: 0800 17 27 43
- International: +27 11 815 60 15 +27 82 775 33 05

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance
EU-GHS / CLP
Hazard Class(es) / Hazard Class- and Category Code(s)
Flammable liquid
Acute toxicity
Serious eye irritation
Skin irritation
Specific target organ toxicity – repeated exposure

EU-DSD / DPD
Indication(s) of danger and risk phrase(s)
Highly flammable
Harmful
Irritant

2.2 Label elements
EU-GHS / CLP
Hazard pictogram(s)

Signal word: Danger
Hazard statement(s):
H225: Highly flammable liquid and vapour
H332: Harmful if inhaled.
H315: Causes skin irritation.
H319: Causes serious eye irritation.

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09-02-2011
Pagina 1 van 7
Safety data sheet  
according to Regulation (EC) No 453/2010

**Diacetyl**

| H335 | May cause respiratory irritation. |
| Precautory statements |  |
| P210 | Keep away from heat / sparks / open flames / hot surfaces – No smoking. |
| P233 | Keep container tightly closed. |
| P241 | Use explosion-proof electrical lighting and equipment. |
| P242 | Use only non-sparking tools. |
| P243 | Take precautions against static discharge. |
| P260 | Do not breathe vapours. |
| P264 | Wash hands thoroughly after handling. |
| P270 | Do not eat, drink or smoke when using this product. |
| P271 | Use only outdoors or in a well-ventilated area. |
| P301 + P312 | IF SWALLOWED: Call a POISON CENTER or doctor / physician if you feel unwell. |
| P302 + P352 | IF ON SKIN: Wash with plenty of soap and water. |
| P304 + P340 | IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. |
| P305 + P351 + P 338 | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. |
| P312 | Call a POISON CENTER or doctor / physician if you feel unwell. |
| P330 | Rinse mouth. |
| P332 + P313 | If skin irritation occurs: Get medical advice / attention. |
| P337 + P313 | If eye irritation persists: Get medical advice / attention. |
| P370+P378 | In case of fire: Use powder, alcohol-resistant foam, water spray, carbon dioxide for extinction. |
| P403 + P233 | Store in a well-ventilated place. Keep container tightly closed. |
| P501 | Disposal: Dispose of contents / container to a specialised waste disposal plant in accordance with local / regional regulations. |

2.3 Other hazards  
Not applicable.

3. **COMPOSITION / INFORMATION ON INGREDIENTS**

<table>
<thead>
<tr>
<th>Main constituent</th>
<th>Identity</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,3-Butanedione</td>
<td>CAS-No.</td>
<td>431-03-8</td>
</tr>
<tr>
<td></td>
<td>EC-No.</td>
<td>207-069-8</td>
</tr>
</tbody>
</table>

4. **FIRST AID MEASURES**

4.1 Description of first aid measures

**Inhalation**  
Fresh air, rest. Get medical advice / attention if you feel unwell.

**Skin contact**  
Remove contaminated clothes, rinse skin with water or shower. If skin irritation occurs: Get medical advice / attention.

**Eye contact**  
First rinse with plenty of water (remove lenses if possible). If eye irritation persists: Get medical advice / attention.

**Ingestion**  
Rinse mouth. Get medical advice / attention if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed

**Acute symptoms and effects**  
May cause damage to lung by brief exposure to high concentrations.  
Serious eye irritation.  
Skin and respiratory irritation.

**Delayed symptoms and effects**  
May cause damage to lung through prolonged or repeated exposure.

4.3 Indication of any immediate medical attention and special treatment needed  
Not applicable.

5. **FIREFIGHTING MEASURES**

5.1 Extinguishing media  
Alcohol-resistant foam, carbon dioxide, powder, water spray.
Diacetyl

1. IDENTIFICATION OF THE SUBSTANCE AND OF THE COMPANY

1.1 Product identifier

Chemical name: 2,3-Butanedione
Synonyms: Butanidine, Butane-2,3-dione, 2,3-Butadione, Bioacety, Dimethyl diketone, 2,3-Dimethyl glycolal.

Formula: C₆H₁₂O₂
Molecular mass: 86.09
FL-No.: 07.052
CAS-No.: 431-03-8
FEMA-No.: 2370
EC-No.: 207-069-8
Annex VI No.: –

1.2 Relevant identified uses of the substance and uses advised against

Flavouring agent.

1.3 Details of the supplier of the safety data sheet

Manufacturer: Illovo Sugar (South Africa) Limited
Address: Gleneagles Park no. 3C
Mount Edgecombe
4300 South Africa
Telephone number: +27 31 508 43 00
Telefax number: +27 31 508 43 10
E-mail address: treed@illovo.co.za

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Serious eye irritation
Skin irritation
Specific target organ toxicity – repeated exposure

EU-DSD / DPD
Indication(s) of danger and risk phrase(s):
Highly flammable
Harmful
Irritant

2.2 Label elements

EU-GHS / CLP
Hazard pictogram(s):

Signal word: Danger

Hazard statement(s):
H225
Highly flammable liquid and vapour
H373
May cause damage to organs (lung) through prolonged or repeated exposure.
H302
Harmful if swallowed.
H332
Harmful if inhaled.
H315
Causes skin irritation.
H319
Causes serious eye irritation.
Diacetyl

**Precautionary statements**
- P210: Keep away from heat / sparks / open flames / hot surfaces – No smoking.
- P233: Keep container tightly closed.
- P241: Use explosion-proof electrical lighting and equipment.
- P242: Use only non-sparking tools.
- P243: Take precautionary measures against static discharge.
- P260: Do not breathe vapours.
- P264: Wash hands thoroughly after handling.
- P270: Do not eat, drink or smoke when using this product.
- P271: Use only outdoors or in a well-ventilated area.
- P280: Wear protective gloves / protective clothing / eye protection protection.
- P301 + P312: IF SWALLOWED: Call a POISON CENTER or doctor / physician if you feel unwell.
- P302 + P352: IF ON SKIN: Wash with plenty of soap and water.
- P304 + P340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
- P305 + P351 + P 338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
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- P332 + P313: If skin irritation occurs: Get medical advice / attention.
- P337 + P313: If eye irritation persists: Get medical advice / attention.
- P370+378: In case of fire: Use powder, alcohol-resistant foam, water spray, carbon dioxide for extinction.
- P403 + P233: Store in a well-ventilated place. Keep container tightly closed.
- P501: Disposal: Dispose of contents / container to a specialised waste disposal plant in accordance with local / regional regulations.

**Other hazards**
Not applicable.

### 3. COMPOSITION / INFORMATION ON INGREDIENTS

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<thead>
<tr>
<th>Main constituent</th>
<th>Identity</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,3-Butanedione</td>
<td>CAS-No. 431-03-8</td>
<td>&gt;98 %</td>
</tr>
<tr>
<td></td>
<td>EC-No. 207-068-8</td>
<td></td>
</tr>
</tbody>
</table>

### 4. FIRST AID MEASURES

#### 4.1 Description of first aid measures

**Inhalation**: Fresh air, rest. Get medical advice / attention if you feel unwell.

**Skin contact**: Remove contaminated clothes, rinse skin with water or shower. If skin irritation occurs: Get medical advice / attention.

**Eye contact**: First rinse with plenty of water (remove lenses if possible). If eye irritation persists: Get medical advice.

**Ingestion**: Rinse mouth. Get medical advice / attention if you feel unwell.

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

**Acute symptoms and effects**: May cause damage to lung by brief exposure to high concentrations. Serious eye irritation. Skin and respiratory irritation.

**Delayed symptoms and effects**: May cause damage to lung through prolonged or repeated exposure.

#### 4.3 Indication of any immediate medical attention and special treatment needed
Not applicable.

### 5. FIREFIGHTING MEASURES

#### 5.1 Extinguishing media
Alcohol-resistant foam, carbon dioxide, powder, water spray.
Safety data sheet according to Regulation (EC) No 453/2010

Diacetyl

5.2 Special hazards arising from the substance
Brief exposure through inhalation to high concentrations may cause lung disease. Highly flammable liquid and vapour. In case of fire toxic gases are formed (carbon monoxide and/or carbon dioxide).

5.3 Advice for firefighters
Self-contained breathing apparatus.
In case of fire: keep tanks / drums cool by spraying with water.

6. ACCIDENTAL RELEASE MEASURES
6.1 Personal precautions, protective equipment and emergency procedures
Additional ventilation.
Gloves, boots.
Self-contained breathing apparatus.

6.2 Environmental precautions
Do not discharge into sewer, surface water or soil.

6.3 Methods and material for containment and cleaning up
Eliminate all sources of ignition or open fire that may come into contact with the spill. Take up small amounts spilled substance with an inert absorbent. Dispose of as hazardous waste.
Dam in large amounts spilled substance and carefully remove with explosion protected vacuum cleaner; recycle if possible. Take remainder up with an inert absorbent. Dispose of as hazardous waste.

6.4 Reference to other sections
See also the sections 8 and 13.

7. HANDLING AND STORAGE
7.1 Precautions for safe handling
Use only in well-ventilated areas.
Use protective breathing masks until ventilation and other controls are determined to be effective.
Wear suitable protective clothing and gloves.
Keep equipment entirely closed, open equipment only for inspection.
Use explosion protected electrical equipment and lighting.
Take precautionary measures against static discharges.
Keep away from sources of ignition – No smoking.

7.2 Conditions for safe storage, including any incompatibilities
Keep container in a well-ventilated place.
Keep container tightly closed.
Fireproof, separated from oxidants, reducing agents, strong bases and acids.
The substance affects many synthetic materials; store only in original packing.

7.3 Specific end use(s)
If used in food: comply with food safety regulation (HACCP).

8. EXPOSURE CONTROLS / PERSONAL PROTECTION
8.1 Control parameters

<table>
<thead>
<tr>
<th>Limit values</th>
<th>Notation</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 hours (TWA)</td>
<td>Short term (15 min.)</td>
</tr>
<tr>
<td>mg/m³</td>
<td>ppm</td>
</tr>
<tr>
<td>n.d.</td>
<td>n.d.</td>
</tr>
</tbody>
</table>

n.d. = not determined

The exposure limits may be exceeded before the odour is perceived.

8.2 Exposure controls
8.2.1 Appropriate engineering controls
Closed equipment.
Ventilation and local exhaust.
Reduction of the operating temperature.
Safety data sheet
according to Regulation (EC) No 453/2010

**Diacetyl**

Caution to assure that polluted air of the general and local exhaust ventilation does not spread contaminants to other areas in the plant.

8.2.2 Individual protection measures, such as personal protective

a) Eye/face protection

Safety goggles.

b) Skin protection

Hand protection

Gloves butyl rubber 0,7 mm

Breakthrough time > 8 hours

Gloves neoprene 0,75 mm

Breakthrough time > 4 hours

Gloves viton 0,7 mm

Breakthrough time > 8 hours

Other

Protective clothing.

c) Respiratory protection

In case of insufficient local exhaust and/or handling with open equipment: breathing protection with a filter for organic vapours (filter type A -EN141 or NIOSH-approved).

d) Thermal hazards

Not applicable.

8.2.3 Environmental exposure controls

Direct polluted air of the local exhaust ventilation out of the plant in a manner in accordance with environmental regulations.

9.  **PHYSICAL AND CHEMICAL PROPERTIES**

9.1 Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Appearance</td>
<td>Yellowish-green liquid</td>
</tr>
<tr>
<td>Odour</td>
<td>Buttery</td>
</tr>
<tr>
<td>Odour threshold (mg/m3)</td>
<td>0,09</td>
</tr>
<tr>
<td>pH (30% solution)</td>
<td>3,2</td>
</tr>
<tr>
<td>Melting point / freezing point (°C)</td>
<td>-2,4</td>
</tr>
<tr>
<td>Boiling point (°C) at 1013 hPa</td>
<td>89 - 90</td>
</tr>
<tr>
<td>Flash point (°C)</td>
<td>7 (tag closed cup)</td>
</tr>
<tr>
<td>Evaporation rate (ether=1)</td>
<td>Not available</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
<td>Not applicable</td>
</tr>
<tr>
<td>Upper/lower explosive limits (vol%)</td>
<td>2,4 - 13,0</td>
</tr>
<tr>
<td>Vapour pressure at 20 °C (hPa)</td>
<td>52</td>
</tr>
<tr>
<td>Vapour density (air=1)</td>
<td>2,97</td>
</tr>
<tr>
<td>Relative density (water=1)</td>
<td>0,99</td>
</tr>
<tr>
<td>Solubility(ies)</td>
<td></td>
</tr>
<tr>
<td>- Water solubility at 20 °C (g/l)</td>
<td>200</td>
</tr>
<tr>
<td>- Fat solubility</td>
<td>Good</td>
</tr>
<tr>
<td>Partition coefficient (log K octanol/water)</td>
<td>-1,34</td>
</tr>
<tr>
<td>Auto-ignition temperature (°C)</td>
<td>365</td>
</tr>
<tr>
<td>Decomposition temperature</td>
<td>Not available</td>
</tr>
<tr>
<td>Viscosity at 20 °C (mPa.s)</td>
<td>Not available</td>
</tr>
<tr>
<td>Explosive properties</td>
<td>None</td>
</tr>
<tr>
<td>Oxidising properties</td>
<td>None</td>
</tr>
</tbody>
</table>

9.2 Other information

Miscibility with

- Ethanol, ether, propylene glycol.
- Not available

Conductivity (pS/m)

- Not available

Heat of combustion (kJ/kg)

- Not available

10. **STABILITY AND REACTIVITY**

10.1 Reactivity

- Not reactive.

10.2 Chemical stability

- Stable. In case of contact with sunlight decomposition.

10.3 Possibility of hazardous reactions

- In case of strong heat polymerization.

10.4 Conditions to avoid

- Avoid contact with open flames, warm surfaces. Protect against direct sunlight.

10.5 Incompatible materials

- Avoid contact with oxidants, reducing agents, strong bases and acids.
Diacetyl

10.6 Hazardous decomposition products
Upon decomposition emits carbon monoxide, carbon dioxide and/or low molecular weight hydrocarbons.

11. TOXICOLOGICAL INFORMATION
11.1 Information on toxicological effects

Acute toxicity
LD50 (oral, rat) (mg/kg)  1580
LD50 (dermal, rabbit) (mg/kg)  > 5000
LC50 (inhalation, rat, 4 hours) (mg/l)  2,25 – 5,2

Likely routes of exposure
The substance may be absorbed into the body by inhalation of vapour or spray and after ingestion.

Effects from short-term exposure
Harmful by inhalation and if swallowed.
Intermittent and subchronic exposures to occupationally-relevant butanedione concentrations caused lymphocytic bronchitis and bronchiolitis in mice. Lymphocytic bronchitis may be a precursor lesion to obliterative bronchiolitis (OB). (Morgan, 2008)
Even brief exposure through inhalation to high concentrations may cause OB. The loss of pulmonary function associated with this illness is permanent.
Irritating to eyes, skin and respiratory system.

- Inhalation  Sore throat, coughing, dullness, tiredness, unconsciousness.
- Skin  Redness.
- Eyes  Redness, pain.
- Ingestion  Sore throat, abdominal pain.

Effects from long-term exposure
Prolonged exposure to high concentrations may cause lung disease (bronchiolitis obliterans).
May cause sensitization by skin contact. Repeated eye contact may cause conjunctivitis.

12. ECOLOGICAL INFORMATION
12.1 Toxicity
LC50 (fish, 96 hours) (mg/l)  46 - 100
EC50 (Daphnia, 48 hours) (mg/l)  Not available
IC50 (algae, 96 hours) (mg/l)  Not available

12.2 Persistence and degradability
Biodegradability
Readily biodegradable. Decomposes to acetic acid and next to carbon dioxide.

Oxygen demand
- biological (5 days) in gO2/g (BOD5)  Not available
- biological (20 days) in gO2/g (BOD20)  Not available
- chemical in gO2/g (COD)  Not available

12.3 Bioaccumulative potential
BCF (Bioconcentration factor) (conc in organisms / conc. in water)  1.0
Risk of bio accumulation is low (BCF < 500 and log Kow < 4).

12.4 Mobility in soil
Adsorption coefficient (Koc) solid phase / liquid phase  1
Highly mobile

12.5 Results of PBT and vPvB assessment
Not available

12.6 Other adverse effects
Ozone depletion potential (ODP) (CCl3F = 1)  Not applicable
Photochemical ozone creation potential (C2H4 = 1)  Not available
Global warming potential (GWP) (CO2 = 1)  Not applicable
Water hazard class (WGK Germany)  2 (hazardous to water)
13 DISPOSAL CONSIDERATIONS
13.1 Waste treatment methods
Recycling by distillation.
Removal to an authorized waste incinerator for solvents or as chemical waste in accordance with local regulations. Do not discharge wastewater into sewer. 07 01 04

European waste list (EURAL)

14 TRANSPORT INFORMATION
14.1 UN No. 2346
14.2 UN proper shipping name BUTANEDIONE
14.3 Transport hazard class(es) 3
14.4 Packinggroup II
14.5 Environmental hazards
Marine pollutant No

14.6 Specials precautions for user
Risk label(s) 3
Tunnel category (D/E)
Hazard Identification Number (Kemier code) 33
ERICard 3-09
Emergency Schedules (EmS)
- Fire schedule Alfa (F-E)
- Spillage schedule Alfa (S-D)

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code
Ship type required Not available
Pollution category Not available

15 REGULATORY INFORMATION
15.1 Safety, health and environmental regulations/legislation specific for the substance
Not available.

15.2 Chemical safety assessment
A Chemical Safety Assessment has not been carried out for butanedione.

16 OTHER INFORMATION
Changes to the previous version.
Classification and labelling according to Regulation (EC) No 453/2010.

Abbreviations and acronyms
DNEL Derived No Effect Level
DMEL Derived Minimal Effect Level
DSD / DPD Dangerous Substances Directive / Dangerous Preparations Directive
EC50 Effect Concentration, 50 percent
ERIC Emergency Response Intervention Card
GHS / CLP Globally Harmonised System / Classification, Labelling and Packaging
IC50 Inhibitory Concentration, 50 percent
LC50 Lethal Concentration, 50 percent
LD50 Lethal Dose, 50 percent
PBT Persistent, Bioaccumulative and Toxic
PNEC Predicted No Effect Concentration
TOD Total Oxygen Demand
TWA Time Weighted Average
vPvB very Persistent and very Bioaccumulative

Literature references and sources for data
Joint FAO/WHO Expert Committee on Food Additives;
W. Auttachato e.a., Diacetyl induces contact sensitization in mice, Abstract No. 1153, NC. Society of Toxicologie; Chemical Information Review Document for Artificial Butter Flavoring (support to the National Toxicology Program), Integrated Laboratory Systems, Inc., January 2007.
Diacetyl

Full text of indication(s) of danger, R phrases and safety advise which are not written out in full under Sections 2 to 15

R11 H111 Highly flammable.
R48/20 H307/36/37/38 Harmful: danger of serious damage to health by prolonged exposure through inhalation (lung disease).
R20/22 H303 Harmful by inhalation and if swallowed.
R36/37/38 H315 Irritating to eyes, respiratory system and skin.

This data sheet has been compiled by KWA. Despite the careful attention paid to the setting up of the text, KWA cannot be held responsible for any error appearing in the text and resulting in whatever damage it may cause.

KWA, Spijksedijk 18c, 4207 GN Gorinchem, Phone +31 183 648 556
2,3-BUTANEDIONE

Date of Peer Review: April 2009

Diacetyl
Dimethylglyoxal
Dimethyl diketone
2,3-Diketobutane
Butanedione

CAS #: 431-03-8
RTECS #: EK2625000
UN #: 2346
EC/EINECS #: 207-069-8

CH$_2$COCOCH$_3$ / C$_4$H$_6$O$_2$
Molecular mass: 86.1

<table>
<thead>
<tr>
<th>TYPES OF HAZARD / EXPOSURE</th>
<th>ACUTE HAZARDS / SYMPTOMS</th>
<th>PREVENTION</th>
<th>FIRST AID / FIRE FIGHTING</th>
</tr>
</thead>
<tbody>
<tr>
<td>FIRE</td>
<td>Highly flammable.</td>
<td>NO open flames, NO sparks, and NO smoking.</td>
<td>Powder, alcohol-resistant foam, water spray, carbon dioxide.</td>
</tr>
<tr>
<td>EXPLOSION</td>
<td>Vapour/air mixtures are explosive.</td>
<td>Closed system, ventilation, explosion-proof electrical equipment and lighting.</td>
<td>In case of fire: keep drums, etc., cool by spraying with water.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EXPOSURE</th>
<th>PREVENT GENERATION OF MISTS!</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Ventilation, local exhaust, or breathing protection.</td>
</tr>
<tr>
<td></td>
<td>Fresh air, rest. Refer for medical attention.</td>
</tr>
<tr>
<td>Skin</td>
<td>Redness.</td>
</tr>
<tr>
<td></td>
<td>Protective gloves. Protective clothing.</td>
</tr>
<tr>
<td></td>
<td>Remove contaminated clothes. Rinse skin with plenty of water or shower.</td>
</tr>
<tr>
<td>Eyes</td>
<td>Redness. Pain. Burns</td>
</tr>
<tr>
<td></td>
<td>Safety goggles or eye protection in combination with breathing protection.</td>
</tr>
<tr>
<td></td>
<td>First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then take to a doctor.</td>
</tr>
<tr>
<td>Ingestion</td>
<td>Sore throat.</td>
</tr>
<tr>
<td></td>
<td>Do not eat, drink, or smoke during work.</td>
</tr>
<tr>
<td></td>
<td>Rinse mouth. Give one or two glasses of water to drink. Seek medical attention if you feel unwell</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>SPILLAGE DISPOSAL</th>
<th>PACKAGING &amp; LABELLING</th>
</tr>
</thead>
<tbody>
<tr>
<td>Remove all ignition sources. Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Do NOT let this</td>
<td></td>
</tr>
</tbody>
</table>

inchem.org/documents/.../eics1168.htm
<table>
<thead>
<tr>
<th>EMERGENCY RESPONSE</th>
<th>STORAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>NFPA Code: H2; F3; R0</td>
<td>Fireproof. Store in an area without drain or sewer access. Separated from: See Chemical Dangers.</td>
</tr>
</tbody>
</table>

IPCS
International Programme on Chemical Safety

Prepared in the context of cooperation between the International Programme on Chemical Safety and the Commission of the European Communities © IPCS, CEC 2005

SEE IMPORTANT INFORMATION ON BACK
2,3-BUTANEDIONE

ICSC: 1168

IMPORTANT DATA

PHYSICAL STATE; APPEARANCE:
GREEN TO YELLOW LIQUID

PHYSICAL DANGERS:
The vapour is heavier than air and may travel along the ground; distant ignition possible.

CHEMICAL DANGERS:
Heating may cause violent combustion or explosion.
Reacts violently with strong acids strong bases and oxidants

OCCUPATIONAL EXPOSURE LIMITS:
TLV not established. MAK not established.

ROUTES OF EXPOSURE:
The substance can be absorbed into the body by inhalation and by ingestion.

INHALATION RISK:
No indication can be given about the rate in which a harmful concentration in the air is reached on evaporation of this substance at 20°C.

EFFECTS OF SHORT-TERM EXPOSURE:
The substance is severely irritating to the eyes. The substance is irritating to the skin and the respiratory tract. The substance may cause effects on the central nervous system lungs and respiratory tract. Exposure at high levels could cause lowering of consciousness.

EFFECTS OF LONG-TERM OR REPEATED EXPOSURE:
Lungs may be affected by repeated or prolonged exposure to the vapour, resulting in impaired functions. SEE NOTES

PHYSICAL PROPERTIES

Boiling point: 88°C
Melting point: -2.4°C
Relative density (water = 1): 1.1
Solubility in water: at 25 °C 20 g/100 ml
Vapour pressure, kPa at 25°C: 7.6
Relative vapour density (air = 1): 3

Relative density of the vapour/air-mixture at 20°C (air = 1):
0.99
Flashpoint: 6°C c.c.
Auto-ignition temperature: 365°C
Explosive limits, vol% in air: 2.4-13 vol%
Octanol/water partition coefficient as log Pow: -1.34

ENVIRONMENTAL DATA

The substance is harmful to aquatic organisms.

NOTES

Irreversible obstructive lung disease has been documented among workers exposed in a variety of settings. These include 2,3-butanedione (diacetyl) production in the chemical industry, production of 2,3-butanedione (diacetyl)-containing flavorings, and production of diacetyl-containing, butter-flavored food products such as microwave popcorn. Many cases have been confirmed to have severe clinical bronchiolitis obliterans. Environmental effects from the substance have not been investigated adequately. Do NOT take working clothes home.

ADDITIONAL INFORMATION

LEGAL NOTICE
Neither the CEC nor the IPCS nor any person acting on behalf of the CEC or the IPCS is responsible for the use which might be made of this information

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See Also:
Toxicological Abbreviations

inchem.org/documents/.../eics1168.htm

3/3
Report – Study on the acute inhalation toxicity $\text{LC}_{50}$ of diacetyl FCC as a vapor in rats 4-hour exposure

DEEMED CONFIDENTIAL
Exposure Simulation to Diacetyl from Popcorn by
Dr. Su-Jung (Candace) Tsai and Dr. Michael Ellenbecker -

DEEMED CONFIDENTIAL
Consumer safety estimate for inhalation of synthetic butter flavoring component of microwave-ready popcorn –

DEEMED CONFIDENTIAL