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FACSIMILE MESSAGE

TO: Glenn Roberts

FROM: Christen Sachse-Vasquez

DATE: 10/5/01

RE: Diacetyl FFIDS

Number of pages including cover sheet: 9

The first FFIDS I am sending you was published in Volume II, 1985. This FFIDS has *not* been updated. The second FFIDS I am sending you was *generated* from the information on the Diacetyl material page of the database. It does not include any toxicological data but it does include the applicable R&S phrases.

I hope this information can be of some assistance.

Thank you,

A handwritten signature in black ink, appearing to read "Christen Sachse-Vasquez", written over a horizontal line.

Christen Sachse-Vasquez

FLAVOR OR FRAGRANCE
INGREDIENT DATA SHEET

I. IDENTIFICATION

1. Chemical Name: Diacetyl
2. CAS Registry Number: 431-03-8 Environ Accession Number: 0227
3. Synonyms: Biacetyl; 2,3-Butanedione; 2,3-Diketobutane; Dimethyl diketane; Dimethylglyoxal [RIFM]; Butadione; Glyoxal, dimethyl- [RTEC]
4. Molecular Formula: C₄H₆O₂ [MER]
5. Molecular Weight: 86.09 [MER]; 86.1 [RTEC, SAX, HCS, SLR]

II. PHYSICAL DATA

1. Boiling Point (760 mm Hg): 87°C-88°C [SLR]; 88°C [SAX, IHS, HCS, KOD, PFP, IND]
2. Melting Point: -3°C [HCS, SLR]; -5.5°C to -3.5°C [KOD]
3. Solubility in H₂O (% by wt. at 20°C): 25 [MER, IHS]; Good [HCS]; Appreciable [KOD]; Soluble [SLR]
4. Solubility in lipids (partition coefficient): Miscible [SLR]
5. Specific Gravity (H₂O = 1): 0.9734 (at 22°C) [PFP]; 0.98 [HCS]; 0.99 (at 15°C/15°C) [MER, KOD]; 0.99 [IHS]; 0.9904 (at 15°C/15°C) [SAX]; 0.979-0.985; 0.98 [KOD]
6. Vapor Pressure (at 20°C): NF
7. Vapor Density (air = 1): 3.0 [SAX, IHS, KOD]
8. Evaporation Rate (Butyl acetate = 1): > 1 [IHS]
9. Flash Point and Method: 5°C (no method reported) [HCS]; 27°C (no method reported) [KOD]; 50°F (no method reported) [IHS]; 80°F (no method reported) [SAX]; 48 F;CC [IND]
10. Flammable Limits in Air (% by Volume) Lower: 2.4 [KOD] Upper: NF

NF = NOT FOUND

1825c/090285

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RIFM 3225

Diacetyl
CAS No. 431-03-8

11. Appearance and Odor: Intensely yellow or yellow-green mobile liquid with a very powerful and diffusive pungent buttery odor [SLR]. The vapors have a chlorine-like odor [MER]

Odor Threshold = 8.6 ppb [RIFM]

III. PHYSICAL HAZARDS

1. NFPA Code: None established

Flammable; vapor is heavier than air and may travel along the ground; distant ignition possible. Dangerous when exposed to heat or flame [SAX]. Due to low electrical conductivity, the substance can generate electrostatic charges as a result of flow, agitation, etc. [HCS]

2. Incompatibility (Materials to Avoid): Strong oxidizers [KOD]
3. Hazardous Decomposition Products: Thermal decomposition or burning may produce carbon monoxide and/or carbon dioxide [KOD]
4. Hazardous Polymerization Potential: Will not occur [IHS, KOD]

IV. HUMAN HEALTH EFFECTS DATA

1. Known Effects of Acute Exposure (Toxicological and Pathological Data)

Ingestion: Sore throat; abdominal pain; may be absorbed [HCS]

Inhalation: Harmful [IHS]. Sore throat, coughing; may be absorbed [HCS]. High concentrations may cause irritation of respiratory tract; capable of producing systemic toxicity [KOD]

Skin Contact: 2% in petrolatum, 48 hr. closed patch test: no irritation or sensitization reactions [TDS]. 2% in petrolatum, no duration reported: no sensitization or irritation [RIFM]. Sensitization reactions [TDS]. Redness [HCS]

Skin Absorption: Can be absorbed through intact skin in toxic amounts [KOD]

Eye Contact: Redness, pain [HCS]. Irritation and transient injury [KOD]

2. Known Effects of Repeated or Prolonged Exposure: Prolonged skin contact may cause irritation [KOD]

V. LABORATORY ANIMAL TOXICOLOGICAL DATA

1. LD₅₀ Data and Associated Pathology

LD₅₀ Oral: 990 mg/kg (g. pig) [RTEC, SAX, RIFM]: ataxia, gasping and coma, with death occurring within a few minutes to 4 days [SLR]. 1580 mg/kg (rat) [MER, RTEC, SAX, RIFM]: depression followed by convulsions within 10-15 min. [SLR]. 1600-3200 mg/kg (rat) [KOD]. 3.0 g/kg, 20% solution (rat, female) [SLR]. 3.4 g/kg, 20% solution (rat, male) [SLR]

LC₅₀ Inhalation: NF

LD₅₀ Dermal: NF

2. Other Acute Toxicity Data (Dose, Duration and Pathology)

Oral: NF

Inhalation: 27 mg/l, 6 hr. (rat): death. 3.5 mg/l, 6 hr. (rat): labored breathing and gasping; weight gain following termination of exposure [KOD]

Dermal: 10 ml/kg, under occlusion (g. pig): death within 48 hr. 1 ml/kg (g. pig): failed to gain original weight during 14-day observation period [KOD]. 5, 10, and 20 ml/kg (separate study from preceding datum) (g. pig): no deaths; at 10 and 20 ml/kg, animals failed to gain original weight. 100% concentration, dropped directly on skin, uncovered (g. pig): slight irritation [KOD]

500 mg, 24 hr. (rabbit): moderate irritation [RTEC, SAX]. Full strength, 24 hr. under occlusion (rabbit): moderate irritation [RIFM, TDS]

Eye: 1 drop (rabbit): immediate irritation; tissue damage [KOD]

Other: 350 mg/kg, intraperitoneal injection (mouse): maximum tolerated dose by mice previously given six intraperitoneal injections over a 2-wk. period. 500 mg/kg, intraperitoneal injection (rat): uncoupled oxidative phosphorylation was observed in rat liver mitochondria [RIFM]

NF = NOT FOUND

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3. Subchronic/Chronic Toxicity Data (Dose, Duration and Pathology)

Oral: 10, 30, and 90 mg/kg/day, 90 days, intubation (rat): no adverse effects [RIFM]. 540 mg/kg/day, 90 days, intubation (rat): decrease in weight gain at wk. 4 in both sexes (more pronounced in males); a decrease in hemoglobin and hematocrit at wk. 7-13; increased water consumption; anaemia; increased reticulocyte and leucocyte count; and increased relative weights of the liver, kidneys, adrenal and pituitary glands; at autopsy, stomach lesions showed ulceration and necrosis, with infiltration by inflammatory cells in 15/15 males and 14/15 females [RIFM, SLR, TDS]

Inhalation: NF

Dermal: NF

Eye: NF

4. Reproductive Toxicity (Includes Teratogenesis)

Oral: < 1.6 starter distillate, 10 consecutive days during gestation, intubation (mouse, rat, and hamster): no effect on maternal or fetal survival or nidation; number of fetal abnormalities was not significant when compared to control animals [RIFM, TDS]

Inhalation: NF

Dermal: NF

Other: NF

5. Carcinogenesis

Oral: NF

Inhalation: NF

Dermal: NF

Other: TDL₀ = 1700 mg/kg, 8 weeks, intermittent administration, intraperitoneal (mouse): equivocal tumorigenic agent by RTECs criteria; tumors in lungs, thorax, or respiratory tract [RTEC, SAX]. 1.7 and 8.4 g/kg, 3 times/wk., 8 wk., intraperitoneal injection (mouse): number of pulmonary tumors in treated mice after 24 wk. did not differ significantly from the control values [RIFM]

NF = NOT FOUND

6. Mutagenesis

In Vitro: Mutation in Microorganisms (*Salmonella typhimurium*): 1 mg/plate; mutation data [RTEC]. Mutation in Microorganisms (tissue unspecified): starter distillate; not genetically active [RIFM]. Mutation in Mammalian Somatic Cells (tissue unspecified): starter distillate; not genetically active [RIFM]

In Vivo: Other mutation system (human - embryo): 20 mg/l; mutation data [RTEC]

VI. OCCUPATIONAL EXPOSURE GUIDELINES

1. OSHA PEL (and rationale): ppm mg/m³ Date:

None established

2. ACGIH TLV: ppm mg/m³ Date:

None established

VII. Other Information

Council of Europe evaluation was Approval

Food and Drug Administration evaluation was GRAS Affirmed As a flavoring agent and adjuvant at levels consistent with current GMP.

Flavoring Extract Manufacturer's Association evaluation was GRAS

VIII. Statements Relevant to Making a Health Hazard Determination

Irritation Data Liquid and vapor may be irritating to skin and eyes.

Vapor is irritating to throat and lungs.

NF = NOT FOUND

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FLAVOR OR FRAGRANCE INGREDIENT DATA SHEET

Diacetyl

CAS Registry Number 431-03-8

I. IDENTIFICATION

1. Chemical Name: Diacetyl
2. CAS Registry Number: 431-03-8
3. Synonyms: Biacetyl; 2,3-Butanedione; 2,3-Diketobutane; Dimethyl diketone; Dimethylglyoxal
4. Molecular Formula: C₄H₆O₂
5. Molecular Weight: 86.09
6. FEMA Number: 2370 RIFM Computer ID Number: 890

II. PHYSICAL DATA

1. Boiling Point: 88~C [Bowles,1998]
2. Flash Point: 48°F;CC [FMA]
3. Log KOW (calculated): -1.34 [Syracuse Research Corp.]
4. Melting Point: Not Found
5. Solubility in Water: Not Found
6. Specific Gravity: 0.981 [FMA]
7. Vapor Pressure: Not Found
8. Appearance and Odor: Merck Index (1976)

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Research Institute for Fragrance Materials, Inc. and
Fragrance Materials Association of the United States, Inc
Flavor and Extract Manufacturers' Association of the United States, Inc.

Diacetyl
CAS Registry Number 431-03-8

III. PHYSICAL HAZARDS

1. NFPA Code: None established
2. Incompatibility (Materials to Avoid): Not found
3. Hazardous Decomposition Products: Not found
4. Hazardous Polymerization Potential: Not found

IV. HUMAN HEALTH EFFECTS DATA

Known Effects of Acute Exposure (Toxicological and Pathological Data)

Ingestion: Not Found

Inhalation: Not Found

Skin Contact: Not Found

Skin Absorption: Not Found

Eye Contact: Not Found

V. LABORATORY ANIMAL TOXICOLOGICAL DATA

Not Found

VI. OCCUPATIONAL EXPOSURE GUIDELINES

Not Found

VII. ADDITIONAL INFORMATION

Canadian Domestic Substances List: Registered

European Inventory of Existing Commercial Chemical Substance: Registered as 207-069-8

TSCA Inventory List: Registered

Council of Europe: A - may be used in foodstuffs

Food and Drug Administration: GRAS Affirmed as a flavoring agent and adjuvant at levels consistent with current GMP and with specifications.

Flavor and Extract Manufacturers' Association: Generally Recognized as Safe as a flavor ingredient - GRAS 3.

Indicative Non-Exhaustive List: Listed

Joint Expert Committee on Food Additives: No ADI allocated. Specifications

VIII. STATEMENTS RELEVANT TO MAKING A HEALTH HAZARD DETERMINATION

Irritation Data Vapor is irritating to throat and lungs.

Liquid and vapor may be irritating to skin and eyes.

IX. CLASSIFICATION AND LABELING AS PRESCRIBED IN ANNEX I TO THE DANGEROUS SUBSTANCES DIRECTIVE 67/548/EEC OR IN ANNEX VI OF THIS DIRECTIVE AS DETERMINED BY THE IFRA/IOFI/EFFA WORKGROUP

S26 In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

R41 Risk of serious damage to eyes.

R39 Danger of very serious irreversible effects.

R38 Irritating to skin.

R20 Harmful by inhalation.

Disclaimer: All listed Risk and Safety statements are suggested by the IFRA/IOFI/EFFA Labeling Group. Final confirmation of these phrases can be found in the most recent Labeling Manual (formerly issued as an IFRA and IOFI Information Letter). Members with access to the RIFM/FEMA Database can obtain all confirmed statements.