

SECTION 1: Identification

1.1. Identification

Product form : Substance
 Trade name : R-1,3-BUTANEDIOL
 Chemical name : (R)-(-)-butane-1,3-diol
 IUPAC name : butane-1,3-diol
 CAS-No. : 6290-03-5
 Formula : C4H10O2
 Synonyms : 1,3-Butanediol, (R)-; 1,3-Butanediol, (3R)-; BUTANE-1,3-DIOL, (R)-(-)-

1.2. Recommended use and restrictions on use

Use of the substance/mixture : For use as a direct food additive in beverages, bars and gels for human consumption

1.3. Supplier

Supplier:
 Genomatica
 4757 Nexus Center Drive
 San Diego, CA 92121, USA
 +1 (858) 824-1771
 safety@genomatica.com

Manufacturer:
 XSTO Solutions, LLC
 145 P. Rickman Industrial Drive, Suite 200
 Canton, GA 30115

1.4. Emergency telephone number

Emergency number : For product information call: +1 858-824-1771
 For Hazardous Materials [or Dangerous Goods] Incident, Spill, Leak, Fire, Exposure, or Accident call ChemTel (MIS9359661) by dialing 1-800-255-3924 or +1-813-248-0585 for callers outside US territories and Canada.

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS US classification

Not classified

2.2. GHS Label elements, including precautionary statements

GHS US labeling

No labeling applicable

2.3. Other hazards which do not result in classification

No additional information available

2.4. Unknown acute toxicity (GHS US)

Not applicable

SECTION 3: Composition/Information on ingredients

3.1. Substances

Name	Product identifier	%	GHS US classification
R-1,3-Butanediol (Main constituent)	CAS-No.: 6290-03-5	99 – 100	Not classified

3.2. Mixtures

Not applicable

SECTION 4: First-aid measures

4.1. Description of first aid measures

- First-aid measures after inhalation : Remove victim to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical advice/attention.
- First-aid measures after skin contact : Wash skin with plenty of water and soap. Seek medical attention if irritation develops.
- First-aid measures after eye contact : Remove contact lenses if easy to do. Immediately flush eyes thoroughly with water for at least 15 minutes. Seek medical attention if irritation develops.
- First-aid measures after ingestion : Do not induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth out with water. In all cases of doubt, or when symptoms persist, seek medical attention.

4.2. Most important symptoms and effects (acute and delayed)

- Symptoms/effects : Not expected to present a significant hazard under anticipated conditions of normal use.

4.3. Immediate medical attention and special treatment, if necessary

Treat symptomatically.

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

- Suitable extinguishing media : For small fire: Dry powder. For large fire: Water spray. Water fog. Foam.
- Unsuitable extinguishing media : Do not use water jet.

5.2. Specific hazards arising from the chemical

- Fire hazard : May be combustible at high temperature.
- Explosion hazard : None known.
- Hazardous decomposition products in case of fire : Carbon dioxide. Carbon monoxide.

5.3. Special protective equipment and precautions for fire-fighters

No additional information available

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

- Protective equipment : Use personal protective equipment as required.
- Emergency procedures : Evacuate unnecessary personnel.

6.1.2. For emergency responders

- Protective equipment : Wear recommended personal protective equipment. For further information refer to section 8: "Exposure controls/personal protection".
- Emergency procedures : Ventilate area.

6.2. Environmental precautions

Prevent entry to sewers and public waters.

6.3. Methods and material for containment and cleaning up

- Methods for cleaning up : For small spills: dilute with small amount of water and mop up, or absorb with an inert dry material and place in an appropriate waste disposal container. Large spills: Contain and/or absorb spill with inert material (sand, vermiculite or other appropriate material), then place in suitable container. Flush residue with large amounts of water. Dispose in a safe manner in accordance with local/national regulations.

6.4. Reference to other sections

For further information refer to section 8: "Exposure controls/personal protection". For disposal of residues refer to section 13: "Disposal considerations".

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
 Hygiene measures : Handle in accordance with good industrial hygiene and safety practice. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Store tightly closed in a dry, cool and well-ventilated place.
 Incompatible materials : Strong oxidizing agents. Acid chlorides. Acid anhydrides. Chloroformates. Reducing agents.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

R-1,3-BUTANEDIOL (6290-03-5)
No additional information available

8.2. Appropriate engineering controls

Appropriate engineering controls : Provide local exhaust or general room ventilation.

8.3. Individual protection measures/Personal protective equipment

Hand protection:

Impermeable protective gloves

Eye protection:

Use eye protection to EN 166, designed to protect against liquid splashes

Skin and body protection:

Wear suitable protective clothing. Chemical resistant suit.

Respiratory protection:

Not required for normal conditions of use. In case of insufficient ventilation, wear suitable respiratory equipment. Approved organic vapor respirator

SECTION 9: Physical and chemical properties**9.1. Information on basic physical and chemical properties**

Physical state	: Liquid
Appearance	: Clear.
Color	: Colorless
Odor	: Odorless
Odor threshold	: No data available
pH	: No data available
Melting point	: No data available
Freezing point	: < -50 °C at 101.3 kPa
Boiling point	: 207.5 °C at 101.3 kPa
Flash point	: 121 °C at 1013 hPa
Relative evaporation rate (butyl acetate=1)	: No data available
Flammability (solid, gas)	: Not applicable.
Vapor pressure	: > 8 - < 10 at 20 °C
Relative vapor density at 20 °C	: No data available
Relative density	: ≥ 1.004 - ≤ 1.006 g/cm ³ at 20 °C
Solubility	: Water: ≈ 999800 mg/l at 25 °C
Partition coefficient n-octanol/water (Log Pow)	: ≥ -0.92 - ≤ -0.08 at 25 °C
Auto-ignition temperature	: 395 °C at 1013 hPa
Decomposition temperature	: No data available
Viscosity, kinematic	: > 96 - < 98 at 25 °C
Viscosity, dynamic	: No data available
Explosion limits	: Not applicable
Explosive properties	: Product is not explosive.
Oxidizing properties	: Non oxidizing material.

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity**10.1. Reactivity**

No dangerous reactions known under normal conditions of use.

10.2. Chemical stability

Stable under use and storage conditions as recommended in section 7.

10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

10.4. Conditions to avoid

No additional information available

10.5. Incompatible materials

Strong oxidizing agents. Acid chlorides. Acid anhydrides. Chloroformates. Reducing agents.

10.6. Hazardous decomposition products

On combustion forms: Carbon oxides (CO, CO₂).

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity (oral)	: Not classified (Based on available data, the classification criteria are not met)
Acute toxicity (dermal)	: Not classified (Based on available data, the classification criteria are not met)
Acute toxicity (inhalation)	: Not classified (Based on available data, the classification criteria are not met)

R-1,3-BUTANEDIOL (6290-03-5)

LD50 oral rat	≈ 22800 mg/kg body weight (results obtained on a similar substance)
Skin corrosion/irritation	: Not classified (Based on available data, the classification criteria are not met)
Serious eye damage/irritation	: Not classified (Based on available data, the classification criteria are not met)
Respiratory or skin sensitization	: Not classified (Based on available data, the classification criteria are not met)
Germ cell mutagenicity	: Not classified (Based on available data, the classification criteria are not met)
Carcinogenicity	: Not classified (Based on available data, the classification criteria are not met)

R-1,3-BUTANEDIOL (6290-03-5)

NOAEL (chronic,oral,animal/male,2 years)	≈ 5000 mg/kg body weight rat (results obtained on a similar substance)
Reproductive toxicity	: Not classified (Based on available data, the classification criteria are not met)

R-1,3-BUTANEDIOL (6290-03-5)

NOAEL (animal/male, F0/P)	≈ 5000 mg/kg body weight rat (results obtained on a similar substance)
STOT-single exposure	: Not classified (Based on available data, the classification criteria are not met)
STOT-repeated exposure	: Not classified (Based on available data, the classification criteria are not met)
Aspiration hazard	: Not classified (Based on available data, the classification criteria are not met)
Viscosity, kinematic	: > 96 - < 98 at 25 °C
Likely routes of exposure	: Inhalation. Ingestion. Eyes. Skin.
Symptoms/effects	: Not expected to present a significant hazard under anticipated conditions of normal use.
Other information	: Due to the extreme structural similarity of (R)-(-)-butane-1,3-diol (CAS No. 6290-03-5) and racemic butane-1,3-diol (CAS No. 107-88-0), the toxicological properties of 1,3 BG are very similar or slightly worse case, and provide a sound basis for a slightly conservative assessment of the hazard profile of R 1,3 BG.

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : Due to the extreme structural similarity of (R)-(-)-butane-1,3-diol (CAS No. 6290-03-5) and racemic butane-1,3-diol (CAS No. 107-88-0), the environmental fate, ecotoxicological properties of 1,3 BG are very similar or slightly worse case, and provide a sound basis for a slightly conservative assessment of the hazard profile of R 1,3 BG.

R-1,3-BUTANEDIOL (6290-03-5)	
LC50 - Fish [1]	> 100 mg/l (based on mortality) (results obtained on a similar substance)
EC50 - Crustacea [1]	> 1000 mg/l (based on mobility) (results obtained on a similar substance)
NOEC chronic crustacea	85 mg/l 21 d - Daphnia magna (based on reproduction) (results obtained on a similar substance)

12.2. Persistence and degradability

R-1,3-BUTANEDIOL (6290-03-5)	
Persistence and degradability	Readily biodegradable.

12.3. Bioaccumulative potential

R-1,3-BUTANEDIOL (6290-03-5)	
Partition coefficient n-octanol/water (Log Kow)	$\geq -0.92 - \leq -0.08$ at 25°C
Bioaccumulative potential	No bioaccumulation.

12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

No additional information available

SECTION 13: Disposal considerations

13.1. Disposal methods

Waste treatment methods : Disposal must be done according to official regulations.
 Product/Packaging disposal recommendations : Handle unclean empty containers as full ones.

SECTION 14: Transport information

In accordance with Department of Transport / Transportation of Dangerous Goods / IMDG / IATA

DOT	TDG	IMDG	IATA
14.1. UN number			
Not regulated for transport			
14.2. Proper Shipping Name			
Not applicable	Not applicable	Not applicable	Not applicable
14.3. Transport hazard class(es)			
Not applicable	Not applicable	Not applicable	Not applicable
14.4. Packing group			
Not applicable	Not applicable	Not applicable	Not applicable
14.5. Environmental hazards			
Not applicable	Not applicable	Not applicable	Not applicable
No supplementary information available			

14.6. Special precautions for user

DOT
No data available

TDG
No data available

IMDG
No data available

IATA
No data available

14.7. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

SECTION 15: Regulatory information

15.1. US Federal regulations

The EPA has identified Reproductive Toxicity as a concern, however this is not classifiable based on GHS criteria.

R-1,3-Butanediol	CAS-No. 6290-03-5	100%
------------------	-------------------	------

This product or mixture is not known to contain a toxic chemical or chemicals in excess of the applicable de minimis concentration as specified in 40 CFR §372.38(a) subject to the reporting requirements of section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 and 40 CFR Part 372.

15.2. International regulations

CANADA

R-1,3-BUTANEDIOL (6290-03-5)

Not listed on the Canadian DSL (Domestic Substances List)/NDSL (Non-Domestic Substances List)

EU-Regulations

No additional information available

National regulations

No additional information available

15.3. US State regulations

California Proposition 65 - This product does not contain any substances known to the state of California to cause cancer, developmental and/or reproductive harm

SECTION 16: Other information

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Data sources	: CSR - Chemical Safety Report.
Other information	: Genomatica fermentatively produces (R)-(-)-butane-1,3-diol (CAS No. 6290-03-5; R-1,3 BG) with a purity of $\geq 99\%$. Due to the extreme structural similarity of R-1,3 BG and the racemic butane-1,3-diol (CAS No. 107-88-0; 1,3 BG) substances, the hazard profile of the two substances are very similar. The physical-chemical properties of 1,3 BG and R-1,3 BG are identical while the environmental fate, ecotoxicological and toxicological properties of 1,3 BG are very similar or slightly worse case, and provide a sound basis for a slightly conservative assessment of the hazard profile of R-1,3 BG.

Safety Data Sheet (SDS), USA

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product. Avela™ (R)-1,3-BUTANEDIOL is the subject of Genomatica's EU and US trademark applications.