

COFFEE BEANS FRAGRANCE

Safety Data Sheet

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

Issue date: 06/01/2020

Revision date: 10/11/2024

Supersedes: 11/11/2020

Version: 1.3

SECTION 1: Identification

1.1. Identification

Product form : Mixture
Product name : COFFEE BEANS FRAGRANCE
CAS-No. : N/A
Product code : 99182

1.2. Recommended use and restrictions on use

1.3. Supplier

Shay and Company
10639 SE Fuller Rd
Milwaukie OR 97222
503-653-1155

1.4. Emergency telephone number

Emergency number : CHEMTREC - USA: 800-424-9300 International: +1 703-527-3887 / 1-800-424-9300
CCN 1014530

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS US classification

Skin sensitization, Category 1 May cause an allergic skin reaction

2.2. GHS Label elements, including precautionary statements

GHS US labeling

Hazard pictograms (GHS US) :



GHS07

Signal word (GHS US) : Warning
Hazard statements (GHS US) : May cause an allergic skin reaction
Precautionary statements (GHS US) : Avoid breathing dust/fume/gas/mist/vapors/spray.
Contaminated work clothing must not be allowed out of the workplace.
Wear protective gloves/protective clothing/eye protection/face protection.
If on skin: Wash with plenty of water.
Specific treatment (see supplemental first aid instruction on this label).
If skin irritation or rash occurs: Get medical advice/attention.
Wash contaminated clothing before reuse.
Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation.

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

Not applicable

3.2. Mixtures

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Name	Product identifier	%	GHS US classification
VANILLIN	(CAS-No.) 121-33-5	5 – 10	Eye Irrit. 2A, H319
(Z)-3,4,5,6,6-Pentamethylhept-3-en-2-one	(CAS-No.) 81786-73-4	1 – 5	Flam. Liq. 4, H227 Skin Sens. 1B, H317
ETHYL VANILLIN	(CAS-No.) 121-32-4	1 – 5	Eye Irrit. 2B, H320
ACETYL CEDRENE	(CAS-No.) 32388-55-9	1 – 5	Skin Sens. 1B, H317
Methylcyclopentenolone	(CAS-No.) 80-71-7	1 – 5	Acute Tox. 4 (Oral), H302
ETHYL MALTOL	(CAS-No.) 4940-11-8	1 – 5	Acute Tox. 4 (Oral), H302
(E)-3,4,5,6,6-Pentamethylhept-3-en-2-one	(CAS-No.) 81786-74-5	0.1 – 5	Flam. Liq. 4, H227 Skin Sens. 1B, H317
4-Hydroxy-2,5-dimethyl-3(2H)-furanone	(CAS-No.) 3658-77-3	0.1 – 1	Acute Tox. 4 (Oral), H302 Skin Corr. 1B, H314 Eye Dam. 1, H318 Skin Sens. 1A, H317

Full text of hazard classes and H-statements : see section 16

SECTION 4: First-aid measures

4.1. Description of first aid measures

- First-aid measures general : If you feel unwell, seek medical advice.
- First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing.
- First-aid measures after skin contact : Wash skin with plenty of water. Take off contaminated clothing. If skin irritation or rash occurs: Get medical advice/attention.
- First-aid measures after eye contact : Rinse eyes with water as a precaution.
- First-aid measures after ingestion : Call a poison center/doctor/physician if you feel unwell.

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

- Symptoms/effects after inhalation : No data available.
- Symptoms/effects after skin contact : May cause an allergic skin reaction.
- Symptoms/effects after eye contact : None under normal conditions.
- Symptoms/effects after ingestion : No data available.

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 : Water spray. Dry powder. Foam. Carbon dioxide.
- Unsuitable extinguishing media : Do not use a heavy water stream.

5.2. Specific hazards arising from the chemical

- Fire hazard : No fire hazard.
- Explosion hazard : No direct explosion hazard.
- Reactivity : The product is non-reactive under normal conditions of use, storage and transport.

5.3. Special protective equipment and precautions for fire-fighters

- Firefighting instructions : Fight fire from safe distance and protected location. Do not enter fire area without proper protective equipment, including respiratory protection.
- Protection during firefighting : Do not attempt to take action without suitable protective equipment. Self-contained breathing apparatus. Complete protective clothing.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

- General measures : Stop leak if safe to do so. Notify authorities if product enters sewers or public waters. Absorb spillage to prevent material-damage.

6.1.1. For non-emergency personnel

- Protective equipment : Wear recommended personal protective equipment.
- Emergency procedures : Ventilate spillage area. Avoid contact with skin and eyes. Avoid breathing dust/fume/gas/mist/vapors/spray.

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6.1.2. For emergency responders

- Protective equipment : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".
- Emergency procedures : Evacuate unnecessary personnel. Stop leak if safe to do so.

6.2. Environmental precautions

Avoid release to the environment.

6.3. Methods and material for containment and cleaning up

- For containment : Absorb spilled material with sand or earth. Contain any spills with dikes or absorbents to prevent migration and entry into sewers or streams. Stop leak, if possible without risk.
- Methods for cleaning up : Take up liquid spill into absorbent material.
- Other information : Dispose of materials or solid residues at an authorized site.

6.4. Reference to other sections

For further information refer to section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

- Additional hazards when processed : Not expected to present a significant hazard under anticipated conditions of normal use.
- Precautions for safe handling : Ensure good ventilation of the work station. Avoid contact with skin and eyes. Avoid breathing dust/fume/gas/mist/vapors/spray. Wear personal protective equipment.
- Hygiene measures : Contaminated work clothing should not be allowed out of the workplace. Wash contaminated clothing before reuse. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

7.2. Conditions for safe storage, including any incompatibilities

- Technical measures : Keep in a cool, well-ventilated place away from heat.
- Storage conditions : Keep cool. Protect from sunlight.
- Packaging materials : Store always product in container of same material as original container.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

OIL, COFFEE BEANS* (N/A)
No additional information available
Methylcyclopentenolone (80-71-7)
No additional information available
ETHYL VANILLIN (121-32-4)
No additional information available
VANILLIN (121-33-5)
No additional information available
ETHYL MALTOL (4940-11-8)
No additional information available
ACETYL CEDRENE (32388-55-9)
No additional information available
(E)-3,4,5,6,6-Pentamethylhept-3-en-2-one (81786-74-5)
No additional information available
(Z)-3,4,5,6,6-Pentamethylhept-3-en-2-one (81786-73-4)
No additional information available
4-Hydroxy-2,5-dimethyl-3(2H)-furanone (3658-77-3)
No additional information available

8.2. Appropriate engineering controls

- Appropriate engineering controls : Ensure good ventilation of the work station.
- Environmental exposure controls : Avoid release to the environment.

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8.3. Individual protection measures/Personal protective equipment

Personal protective equipment:

Wear recommended personal protective equipment.

Hand protection:

Protective gloves

Eye protection:

Chemical goggles or safety glasses

Skin and body protection:

Wear suitable protective clothing

Respiratory protection:

In case of insufficient ventilation, wear suitable respiratory equipment



SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Color	: YELLOW TO AMBER
Odor	: CHARACTERISTIC, MATCHING RETAINER SAMPLE
Odor threshold	: No data available
pH	: No data available
Melting point	: Not applicable
Freezing point	: No data available
Boiling point	: No data available
Flash point	: 117 °C
Relative evaporation rate (butyl acetate=1)	: No data available
Flammability	: Not applicable.
Vapor pressure	: No data available
Relative vapor density at 20°C	: No data available
Relative density	: 0.945 (0.935 – 0.955)
Solubility	: Insoluble.
Partition coefficient n-octanol/water (Log Pow)	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosion limits	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available

9.2. Other information

Refractive index	: 1.461 (1.451 – 1.471)
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SECTION 10: Stability and reactivity

10.1. Reactivity

The product is non-reactive under normal conditions of use, storage and transport.

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10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

10.4. Conditions to avoid

None under recommended storage and handling conditions (see section 7).

10.5. Incompatible materials

No additional information available

10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity (oral) : Not classified

Acute toxicity (dermal) : Not classified

Acute toxicity (inhalation) : Not classified

Methylcyclopentenolone (80-71-7)

ATE US (oral)	1067 mg/kg body weight
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ETHYL VANILLIN (121-32-4)

LD50 oral rat	> 3160 mg/kg body weight Animal: rat, Guideline: OECD Guideline 401 (Acute Oral Toxicity), Remarks on results: other:
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LD50 dermal rat	> 2000 mg/kg body weight Animal: rat, Guideline: OECD Guideline 402 (Acute Dermal Toxicity)
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ATE US (oral)	3000 mg/kg body weight
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VANILLIN (121-33-5)

LD50 oral rat	3300 mg/kg body weight (Equivalent or similar to OECD 401, Rat, Male / female, Experimental value, Oral, 14 day(s))
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LD50 dermal rat	> 2000 mg/kg body weight (OECD 402: Acute Dermal Toxicity, 24 h, Rat, Male / female, Experimental value, Dermal, 14 day(s))
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ATE US (oral)	3300 mg/kg body weight
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ATE US (dermal)	2600 mg/kg body weight
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ETHYL MALTOL (4940-11-8)

LD50 oral rat	1220 mg/kg body weight (Equivalent or similar to OECD 401, Rat, Experimental value, Oral)
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LD50 dermal rabbit	> 5000 mg/kg body weight Animal: rabbit, Guideline: OECD Guideline 402 (Acute Dermal Toxicity), Remarks on results: no indication of skin irritation up to the relevant limit dose level
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ATE US (oral)	1200 mg/kg body weight
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ACETYL CEDRENE (32388-55-9)

LD50 dermal rabbit	> 5000 mg/kg body weight Animal: rabbit, Guideline: OECD Guideline 402 (Acute Dermal Toxicity), Remarks on results: other:
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ATE US (oral)	4500 mg/kg body weight
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4-Hydroxy-2,5-dimethyl-3(2H)-furanone (3658-77-3)

ATE US (oral)	1608 mg/kg body weight
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Skin corrosion/irritation : Not classified

Serious eye damage/irritation : Not classified

Respiratory or skin sensitization : May cause an allergic skin reaction.

Germ cell mutagenicity : Not classified

Carcinogenicity : Not classified

Reproductive toxicity : Not classified

STOT-single exposure : Not classified

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STOT-repeated exposure : Not classified

ETHYL MALTOL (4940-11-8)	
NOAEL (oral, rat, 90 days)	≥ 200 mg/kg body weight Animal: rat, Guideline: OECD Guideline 453 (Combined Chronic Toxicity / Carcinogenicity Studies)

Aspiration hazard : Not classified
Viscosity, kinematic : No data available
Symptoms/effects after inhalation : No data available.
Symptoms/effects after skin contact : May cause an allergic skin reaction.
Symptoms/effects after eye contact : None under normal conditions.
Symptoms/effects after ingestion : No data available.

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : The product is not considered harmful to aquatic organisms or to cause long-term adverse effects in the environment.

ETHYL VANILLIN (121-32-4)	
LC50 - Fish [1]	87.6 mg/l Test organisms (species): Pimephales promelas
EC50 - Crustacea [1]	26.2 mg/l Test organisms (species): Daphnia magna
LOEC (chronic)	10 mg/l Test organisms (species): Daphnia magna Duration: '21 d'
NOEC (chronic)	5.9 mg/l Test organisms (species): Daphnia magna Duration: '21 d'

VANILLIN (121-33-5)	
LC50 - Fish [1]	57 mg/l (Equivalent or similar to OECD 203, 96 h, Pimephales promelas, Flow-through system, Fresh water, Experimental value)
EC50 - Crustacea [1]	36.79 mg/l (OECD 202: Daphnia sp. Acute Immobilisation Test, 48 h, Daphnia magna, Static system, Fresh water, Experimental value, GLP)
LC50 - Fish [2]	123 mg/l Test organisms (species): Pimephales promelas
ErC50 algae	120 mg/l (OECD 201: Alga, Growth Inhibition Test, 72 h, Pseudokirchneriella subcapitata, Static system, Fresh water, Experimental value, GLP)
LOEC (chronic)	10 mg/l Test organisms (species): Daphnia magna Duration: '21 d'
NOEC (chronic)	5.9 mg/l Test organisms (species): Daphnia magna Duration: '21 d'

ETHYL MALTOL (4940-11-8)	
LC50 - Fish [1]	> 85 mg/l (OECD 203: Fish, Acute Toxicity Test, 96 h, Oncorhynchus mykiss, Semi-static system, Fresh water, Experimental value)
EC50 - Crustacea [1]	27 mg/l (OECD 202: Daphnia sp. Acute Immobilisation Test, 48 h, Daphnia magna, Static system, Fresh water, Experimental value)
ErC50 algae	7.2 mg/l (OECD 201: Alga, Growth Inhibition Test, 72 h, Pseudokirchneriella subcapitata, Static system, Fresh water, Experimental value, GLP)

ACETYL CEDRENE (32388-55-9)	
LC50 - Fish [1]	3 mg/l (OECD 203: Fish, Acute Toxicity Test, 96 h, Pimephales promelas, Static system, Experimental value, GLP)
EC50 - Crustacea [1]	0.86 mg/l (OECD 202: Daphnia sp. Acute Immobilisation Test, 48 h, Daphnia magna, Static system, Experimental value, GLP)
LC50 - Fish [2]	3 mg/l Test organisms (species): Pimephales promelas
ErC50 algae	> 4.3 mg/l (OECD 201: Alga, Growth Inhibition Test, 96 h, Pseudokirchneriella subcapitata, Static system, Experimental value, GLP)
LOEC (chronic)	0.23 mg/l Test organisms (species): Daphnia magna Duration: '21 d'
NOEC (chronic)	0.087 mg/l Test organisms (species): Daphnia magna Duration: '21 d'

12.2. Persistence and degradability

VANILLIN (121-33-5)	
Persistence and degradability	Readily biodegradable in water.

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ETHYL MALTOL (4940-11-8)

Persistence and degradability	Readily biodegradable in water.
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ACETYL CEDRENE (32388-55-9)

Persistence and degradability	Not readily biodegradable in water.
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12.3. Bioaccumulative potential

VANILLIN (121-33-5)

Partition coefficient n-octanol/water (Log Pow)	1.17 (Experimental value, OECD 107: Partition Coefficient (n-octanol/water): Shake Flask Method, 25 °C)
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Bioaccumulative potential	Low potential for bioaccumulation (Log Kow < 4).
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ETHYL MALTOL (4940-11-8)

Partition coefficient n-octanol/water (Log Pow)	2.9 (Practical experience/observation, OECD 117: Partition Coefficient (n-octanol/water), HPLC method, 25 °C)
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Bioaccumulative potential	Low potential for bioaccumulation (Log Kow < 4).
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ACETYL CEDRENE (32388-55-9)

BCF - Fish [1]	867 – 3920 (OECD 305: Bioconcentration: Flow-Through Fish Test, 28 day(s), Oncorhynchus mykiss, Flow-through system, Fresh water, Experimental value, GLP)
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Partition coefficient n-octanol/water (Log Pow)	5.6 – 5.9 (Experimental value, OECD 117: Partition Coefficient (n-octanol/water), HPLC method)
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Bioaccumulative potential	Potential for bioaccumulation (500 ≤ BCF ≤ 5000).
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12.4. Mobility in soil

VANILLIN (121-33-5)

Organic Carbon Normalized Adsorption Coefficient (Log Koc)	3.438 (log Koc, Experimental value)
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Ecology - soil	Low potential for mobility in soil.
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ETHYL MALTOL (4940-11-8)

Ecology - soil	No (test)data on mobility of the substance available.
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ACETYL CEDRENE (32388-55-9)

Organic Carbon Normalized Adsorption Coefficient (Log Koc)	3.5 – 5.1 (log Koc, OECD 121: Estimation of the Adsorption Coefficient (Koc) on Soil and on Sewage Sludge using High Performance Liquid Chromatography (HPLC), Experimental value, GLP)
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Ecology - soil	Low potential for mobility in soil.
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12.5. Other adverse effects

No additional information available

SECTION 13: Disposal considerations

13.1. Disposal methods

Regional waste regulation	: Disposal must be done according to official regulations.
Waste treatment methods	: Dispose of contents/container in accordance with licensed collector's sorting instructions.
Sewage disposal recommendations	: Disposal must be done according to official regulations.
Product/Packaging disposal recommendations	: Disposal must be done according to official regulations.
Additional information	: Do not re-use empty containers.

SECTION 14: Transport information

Department of Transportation (DOT)

In accordance with DOT

Not regulated

Transportation of Dangerous Goods

Not regulated

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Transport by sea

Not regulated

Air transport

Not regulated

SECTION 15: Regulatory information

15.1. US Federal regulations

Methylcyclopentenolone (80-71-7)

Listed on the United States TSCA (Toxic Substances Control Act) inventory

ETHYL VANILLIN (121-32-4)

Listed on the United States TSCA (Toxic Substances Control Act) inventory

(E)-3,4,5,6,6-Pentamethylhept-3-en-2-one (81786-74-5)

Not listed on the United States TSCA (Toxic Substances Control Act) inventory

(Z)-3,4,5,6,6-Pentamethylhept-3-en-2-one (81786-73-4)

Not listed on the United States TSCA (Toxic Substances Control Act) inventory

4-Hydroxy-2,5-dimethyl-3(2H)-furanone (3658-77-3)

Listed on the United States TSCA (Toxic Substances Control Act) inventory

15.2. International regulations

CANADA

Methylcyclopentenolone (80-71-7)

Listed on the Canadian DSL (Domestic Substances List)

ETHYL VANILLIN (121-32-4)

Listed on the Canadian DSL (Domestic Substances List)

VANILLIN (121-33-5)

Listed on the Canadian DSL (Domestic Substances List)

ETHYL MALTOL (4940-11-8)

Listed on the Canadian DSL (Domestic Substances List)

ACETYL CEDRENE (32388-55-9)

Listed on the Canadian DSL (Domestic Substances List)

(E)-3,4,5,6,6-Pentamethylhept-3-en-2-one (81786-74-5)

Listed on the Canadian DSL (Domestic Substances List)

(Z)-3,4,5,6,6-Pentamethylhept-3-en-2-one (81786-73-4)

Listed on the Canadian DSL (Domestic Substances List)

4-Hydroxy-2,5-dimethyl-3(2H)-furanone (3658-77-3)

Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

No additional information available

National regulations

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VANILLIN (121-33-5)
Listed on the United States TSCA (Toxic Substances Control Act) inventory - Status: Active Listed on INSQ (Mexican National Inventory of Chemical Substances)
ETHYL MALTOL (4940-11-8)
Listed on the United States TSCA (Toxic Substances Control Act) inventory - Status: Active Listed on INSQ (Mexican National Inventory of Chemical Substances)
ACETYL CEDRENE (32388-55-9)
Listed on the United States TSCA (Toxic Substances Control Act) inventory - Status: Active Listed on INSQ (Mexican National Inventory of Chemical Substances)

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

Revision date : 10/11/2024

Full text of H-phrases:

	Combustible liquid
H302	Harmful if swallowed
H314	Causes severe skin burns and eye damage
H317	May cause an allergic skin reaction
H318	Causes serious eye damage
H319	Causes serious eye irritation
H320	Causes eye irritation

SDS US (GHS HazCom 2012)

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.