

SAFETY DATA SHEET

according to the OSHA
Hazard Communication Standard

Version 8.23
Revision Date 07/15/2026
Print Date 07/16/2026

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : EPA 506 Phthalate Mix (7 component)

Product Number : 40077-U

Brand : Supelco

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

Restrictions on use : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-
527-3887 CHEMTREC (International) 24
Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Flammable liquids : Category 2

Skin irritation : Category 2

Reproductive toxicity : Category 1B

Specific target organ toxicity - single exposure : Category 3 (Central nervous system)

Aspiration hazard : Category 1

Short-term (acute) aquatic hazard : Category 1

Long-term (chronic) aquatic hazard : Category 1

Other hazards

None known.

GHS label elements

Hazard pictograms : 

Signal word : Danger

Hazard statements : H225 Highly flammable liquid and vapour.
H304 May be fatal if swallowed and enters airways.
H315 Causes skin irritation.
H336 May cause drowsiness or dizziness.
H360 May damage fertility or the unborn child.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements : **Prevention:**
P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.
P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 Keep container tightly closed.
P240 Ground and bond container and receiving equipment.
P241 Use explosion-proof electrical/ ventilating/ lighting equipment.
P242 Use non-sparking tools.
P243 Take action to prevent static discharges.
P261 Avoid breathing mist or vapours.
P264 Wash skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response:

P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor.

P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.

P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.

P308 + P313 IF exposed or concerned: Get medical advice/ attention.

P331 Do NOT induce vomiting.

P332 + P313 If skin irritation occurs: Get medical advice/ attention.

P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

P391 Collect spillage.

Storage:

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

P403 + P235 Store in a well-ventilated place. Keep cool.

P405 Store locked up.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Mixture

CAS-No. : Not Assigned

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
isooctane	540-84-1*	>= 80 - <= 100	TSC
Benzyl butyl phthalate	85-68-7*	>= 0 - <= 0.1	TSC
dibutyl phthalate	84-74-2*	>= 0 - <= 0.1	TSC
Bis(2-ethylhexyl) phthalate	117-81-7*	>= 0 - <= 0.1	TSC

* Indicates that the identifier is a CAS No.

TSC- the actual concentration or concentration range is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice	: Show this safety data sheet to the doctor in attendance.
If inhaled	: After inhalation: fresh air. Call in physician.
In case of skin contact	: In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.
In case of eye contact	: After eye contact: rinse out with plenty of water. Remove contact lenses.
If swallowed	: After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.
Most important symptoms and effects, both acute and delayed	: The most important known symptoms and effects are described in the labelling (see section 2 GHS label elements) and/or in section 11
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Foam Carbon dioxide (CO ₂) Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible.

Pay attention to flashback.

Vapours are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

Hazardous combustion products	: Carbon oxides
Specific extinguishing methods	: No data available
Further information	: Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	: Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: Wear appropriate personal protective equipment, as indicated in Section 8.
Environmental precautions	: Do not let product enter drains. Risk of explosion.
Methods and materials for containment and cleaning up	: Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2 GHS label elements

Advice on protection against fire and explosion : Keep away from open flames, hot surfaces and sources of ignition.
Take precautionary measures against static discharge.

Advice on safe handling : Work under hood. Do not inhale substance/mixture.
Avoid generation of vapours/aerosols.

Further information on storage conditions : Keep container tightly closed in a dry and well-ventilated place.
Keep away from heat and sources of ignition.
Keep locked up or in an area accessible only to qualified or authorised persons.

Storage class : 3, Flammable liquids

Recommended storage temperature : 36 - 86 °F / 2 - 30 °C

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
isooctane	540-84-1	TWA	300 ppm	ACGIH
dibutyl phthalate	84-74-2	TWA	5 mg/m ³	ACGIH
		TWA	5 mg/m ³	NIOSH REL
		TWA	5 mg/m ³	OSHA Z-1
Bis(2-ethylhexyl) phthalate	117-81-7	TWA	0.1 mg/m ³	ACGIH
		TWA	5 mg/m ³	NIOSH REL
		ST	10 mg/m ³	NIOSH REL
		TWA	5 mg/m ³	OSHA Z-1

Biological occupational exposure limits

Components	CAS-No.	Control parameters	Biological specimen	Sampling time	Permissible concentration	Basis
Bis(2-ethylhexyl) phthalate	117-81-7	Mono(2-ethylhexyl)phthalate	Urine	End of shift	5 µg/g creatinine	ACGIH BEI
		Mono(2-ethyl-5-hydroxyhexyl)phthalate	Urine	End of shift	20 µg/g creatinine	ACGIH BEI
		Mono(2-	Urine	End of	15 µg/g	ACGIH

		ethyl-5-oxohexyl) phthalate		shift	creatinine	BEI
		Mono(2-ethyl-5-carboxyphenyl)phthalate	Urine	End of shift	25 µg/g creatinine	ACGIH BEI

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Remarks : required

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Safety glasses

Skin and body protection : Flame retardant antistatic protective clothing.

Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : liquid

Supelco - 40077-U

Page 7 of 24

Colour	: No data available
Odour	: No data available
Odour Threshold	: No data available
pH	: No data available
Melting point	: No data available
Boiling point/boiling range	: No data available
Flash point	: No data available
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapour pressure	: No data available
Relative vapour density	: No data available
Relative density	: No data available
Density	: No data available
Water solubility	: No data available
Partition coefficient: n- octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available

Explosive properties : Not classified as explosive.
Oxidizing properties : none
Particle characteristics
Particle size : No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity : Vapours may form explosive mixture with air.
Chemical stability : The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions : Violent reactions possible with:
Strong oxidizing agents
Conditions to avoid : Warming.
Incompatible materials : No data available
Hazardous decomposition products : For Hazardous combustion products in the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Mixture

Acute toxicity

Oral: No data available

Acute toxicity estimate Inhalation - 4 h - 25.18 mg/l - vapour(Calculation method)

Acute toxicity estimate Dermal - 2,518 mg/kg
(Calculation method)

Skin corrosion/irritation

Remarks: Mixture causes skin irritation.

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: 2B - Group 2B: Possibly carcinogenic to humans (Bis(2-ethylhexyl) phthalate)

NTP: RAHC - Reasonably anticipated to be a human carcinogen (Bis(2-ethylhexyl)

Supelco - 40077-U

Page 9 of 24

phthalate)

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

May harm the unborn child.

May impair fertility.

Specific target organ toxicity - single exposure

Mixture may cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary oedema and pneumonitis.

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Liver - Irregularities - Based on Human Evidence

Components

isooctane

Acute toxicity

LD50 Oral - Rat - male and female - > 5,000 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - > 33.52 mg/l - vapour

(OECD Test Guideline 403)

Symptoms: mucosal irritations

LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg

(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 24 h

(OECD Test Guideline 404)

Remarks: Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

Respiratory or skin sensitization

Maximisation Test - Guinea pig

Result: negative
(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: TA98

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: human lymphoblastoid cells

Result: negative

Method: OECD Test Guideline 486

Species: Rat - male - Liver cells

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness. - Central nervous system

Acute inhalation toxicity - mucosal irritations

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary oedema and pneumonitis.

Benzyl butyl phthalate

Acute toxicity

LD50 Oral - Rat - male and female - 2,330 mg/kg

(OECD Test Guideline 401)

Inhalation: No data available

LD50 Dermal - Rabbit - > 10,000 mg/kg

Remarks: (RTECS)

Skin corrosion/irritation

Skin - In vitro study

Result: No skin irritation

Remarks: (ECHA)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation - 24 h

Remarks: (ECHA)

Respiratory or skin sensitization

Sensitisation test: - Guinea pig

Result: negative

Remarks: (ECHA)

Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Result: negative

Test Type: sister chromatid exchange assay

Test system: Chinese hamster ovary cells

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Result: negative

Method: US-EPA

Species: Mouse - male - Bone marrow

Result: Positive results were obtained in some in vivo tests.

Method: US-EPA

Species: Mouse - male - Bone marrow

Result: positive

Carcinogenicity

No data available

Reproductive toxicity

May damage the unborn child.

Suspected of damaging fertility.

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure**Aspiration hazard**

No data available

dibutyl phthalate**Acute toxicity**

LD50 Oral - Rat - male and female - 6,279 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - ≥ 15.68 mg/l - aerosol

Remarks: (ECHA)

LD50 Dermal - Rabbit - $> 21,000$ mg/kg

Remarks: (RTECS)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation - 72 h

(OECD Test Guideline 405)

Respiratory or skin sensitization

Maximisation Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Result: negative

Remarks: (ECHA)

Species: Mouse

Result: negative

Remarks: (ECHA)

Carcinogenicity

No data available

Reproductive toxicity

May damage the unborn child.

Suspected of damaging fertility.

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

Aspiration hazard

No data available

Bis(2-ethylhexyl) phthalate

Acute toxicity

LD50 Oral - Rat - 30,000 mg/kg

Remarks: (RTECS)

LC0 Inhalation - Rat - male and female - 4 h - > 10.62 mg/l - vapour

(OECD Test Guideline 403)

Remarks: (highest concentration to be prepared)

LD50 Dermal - Rabbit - 19,800 mg/kg

Remarks: (ECHA)

Skin corrosion/irritation

Skin - Rabbit

Result: slight irritation - 4 h

(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation - 72 h

(OECD Test Guideline 405)

Respiratory or skin sensitization

Maximisation Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

Result: negative

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary cells

Result: negative

Test Type: sister chromatid exchange assay

Test system: Chinese hamster ovary cells

Result: negative

Test Type: Micronucleus test

Test system: Chinese hamster lung cells

Result: negative

Remarks: (ECHA)

Method: OECD Test Guideline 475

Species: Rat - male - Bone marrow

Result: negative

Method: OECD Test Guideline 486

Species: Rat - male and female - Liver cells

Result: negative

Carcinogenicity

This product is or contains a component that has been reported to be possibly carcinogenic based on its IARC, ACGIH, NTP, or EPA classification.

Reproductive toxicity

May damage the unborn child.

May damage fertility.

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

Aspiration hazard

No data available

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

isooctane:

Supelco - 40077-U

Page 14 of 24

Toxicity to fish : LC50 (Oncorhynchus mykiss (rainbow trout)): 0.11 mg/l
End point: mortality
Exposure time: 96 h
Test Type: semi-static test
Analytical monitoring: yes
Method: OECD Test Guideline 203
GLP: yes

Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): 0.4 mg/l
End point: Immobilization
Exposure time: 48 h
Test Type: static test
Analytical monitoring: yes
Remarks: (in analogy to similar products) (ECHA)
The value is given in analogy to the following substances: 2,3,4-Trimethylpentane

M-Factor (Acute aquatic toxicity) : 1

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity) : EC50 (Daphnia magna (Water flea)): 0.23 mg/l
Exposure time: 21 d
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 211
GLP: yes

M-Factor (Chronic aquatic toxicity) : 1

Toxicity to microorganisms : EC0 (Pseudomonas putida): 10,000 mg/l
Remarks: (IUCLID)

Benzyl butyl phthalate:

Toxicity to fish : LC50 (Fish): 0.51 mg/l
End point: mortality
Exposure time: 96 h
Test Type: flow-through test
Analytical monitoring: yes
Remarks: (ECHA)

Toxicity to daphnia and other aquatic invertebrates : LC50 (Americamysis bahia (Mysid)): > 0.74 mg/l
Exposure time: 48 h
Test Type: flow-through test
Analytical monitoring: yes
Method: US-EPA
GLP: yes

Toxicity to algae/aquatic : ErC50 (Desmodesmus subspicatus (green algae)): 1.5

plants	mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes
M-Factor (Acute aquatic toxicity)	: 1
Toxicity to fish (Chronic toxicity)	: NOEC (Pimephales promelas (fathead minnow)): 0.064 - 0.067 mg/l Exposure time: 126 Days Test Type: flow-through test Analytical monitoring: yes Method: US-EPA GLP: yes
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)	: NOEC (Daphnia magna (Water flea)): 0.28 mg/l End point: reproduction rate Exposure time: 21 d Test Type: flow-through test Analytical monitoring: yes Remarks: (ECHA)

Ecotoxicology Assessment

Chronic aquatic toxicity : Very toxic to aquatic life with long lasting effects.

dibutyl phthalate:

Toxicity to fish	: LC50 (Lepomis macrochirus (Bluegill sunfish)): ca. 0.48 mg/l End point: mortality Exposure time: 96 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 203 GLP: yes
Toxicity to daphnia and other aquatic invertebrates	: EC50 (Daphnia magna (Water flea)): ca. 2.99 mg/l End point: mortality Exposure time: 48 h Test Type: static test Analytical monitoring: yes Method: US-EPA GLP: yes
M-Factor (Acute aquatic toxicity)	: 1

Ecotoxicology Assessment

Supelco - 40077-U

Page 16 of 24

Chronic aquatic toxicity : This product has no known ecotoxicological effects.

Bis(2-ethylhexyl) phthalate:

Toxicity to fish	: LC50 (Pimephales promelas (fathead minnow)): > 0.67 mg/l End point: mortality Exposure time: 96 h Test Type: flow-through test Analytical monitoring: yes Method: OECD Test Guideline 203 GLP: yes Remarks: (above the solubility limit in the test medium)
Toxicity to daphnia and other aquatic invertebrates	: EC50 (Daphnia magna (Water flea)): > 0.16 mg/l End point: Immobilization Exposure time: 48 h Remarks: (ECOTOX Database)
Toxicity to algae/aquatic plants	: EC50 (Pseudokirchneriella subcapitata): > 0.003 mg/l Exposure time: 72 h Analytical monitoring: yes Method: OECD Test Guideline 201
Toxicity to fish (Chronic toxicity)	: NOEC (Pimephales promelas (fathead minnow)): 23.8 mg/l Exposure time: 32 d Test Type: flow-through test Remarks: (above the solubility limit in the test medium) (ECOTOX Database)
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)	: NOEC (Daphnia magna (Water flea)): 0.158 mg/l End point: mortality Exposure time: 21 d Test Type: flow-through test Analytical monitoring: yes Method: OECD Test Guideline 211 Remarks: (above the solubility limit in the test medium)
Toxicity to microorganisms	: NOEC (activated sludge): 1,000 mg/l End point: Growth rate Exposure time: 3 h Test Type: static test Method: OECD Test Guideline 209 GLP: yes

Ecotoxicology Assessment

Acute aquatic toxicity : This product has no known ecotoxicological effects.

Chronic aquatic toxicity : This product has no known ecotoxicological effects.

Persistence and degradability

Components:

isooctane:

Biodegradability : aerobic
Inoculum: activated sludge
Concentration: 49 mg/l
Result: Inherently biodegradable.
Biodegradation: 51.3 %
Exposure time: 28 d
Method: OECD Test Guideline 301F

Benzyl butyl phthalate:

Biodegradability : aerobic
Inoculum: activated sludge
Concentration: 100 mg/l
Result: Readily biodegradable.
Biodegradation: 81 %
Exposure time: 14 d
Method: OECD Test Guideline 301C

dibutyl phthalate:

Biodegradability : Inoculum: activated sludge, non-adapted
Concentration: 21.7 mg/l
Result: Readily biodegradable.
Biodegradation: 81 %
Exposure time: 28 d
Method: Regulation (EC) No. 440/2008, Annex, C.4-C
GLP: yes

Bis(2-ethylhexyl) phthalate:

Biodegradability : aerobic
Inoculum: activated sludge, non-adapted
Concentration: 20.3 mg/l
Result: Readily biodegradable.
Biodegradation: ca. 82 %
Exposure time: 29 d
Method: OECD Test Guideline 301B
GLP: yes

Bioaccumulative potential

Components:

isooctane:

Bioaccumulation : Bioconcentration factor (BCF): 231

Partition coefficient: n-octanol/water : log Pow: 4.6
Remarks: Bioaccumulation is not expected.

Benzyl butyl phthalate:

Bioaccumulation : Species: *Lepomis macrochirus*
Bioconcentration factor (BCF): 9.4
Exposure time: 3.27 Days
Temperature: 72 °F / 22 °C
Method: OECD Test Guideline 305

Partition coefficient: n-octanol/water : log Pow: 4.91 (68 °F / 20 °C)
Method: OECD Test Guideline 107
Remarks: Potential bioaccumulation

dibutyl phthalate:

Bioaccumulation : Species: *Pimephales promelas* (fathead minnow)
Bioconcentration factor (BCF): 2,165
Exposure time: 11 d
Concentration: 0.0348 mg/l
Remarks: Does not bioaccumulate.

Partition coefficient: n-octanol/water : log Pow: 4.46 (86 °F / 30 °C)
pH: 5 - 8
Method: Regulation (EC) No. 440/2008, Annex, A.8
Remarks: Potential bioaccumulation

Bis(2-ethylhexyl) phthalate:

Bioaccumulation : Species: *Oncorhynchus mykiss* (rainbow trout)
Bioconcentration factor (BCF): 113
Exposure time: 100 d
Concentration: 0.014 mg/l
Remarks: Does not bioaccumulate.

Mobility in soil

No data available

Other adverse effects

Product:

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances
Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

Components:

isooctane:

Results of PBT and vPvB assessment : Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

Additional ecological information : Biological effects:

Endangers drinking-water supplies if allowed to enter soil and/or waters in large quantities.

Discharge into the environment must be avoided.

Benzyl butyl phthalate:

Additional ecological information : Avoid release to the environment.

Discharge into the environment must be avoided.

dibutyl phthalate:

Additional ecological information : Discharge into the environment must be avoided.

Endocrine disrupting properties

No data available

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No. : UN 1262
Proper shipping name : Octanes solution
Class : 3
Packing group : II
Labels : Class 3 - Flammable liquids
Packing instruction (cargo aircraft) : 364

Packing instruction : 353
(passenger aircraft)

IMDG-Code

UN number : UN 1262
Proper shipping name : OCTANES SOLUTION

Class : 3
Packing group : II
Labels : 3
EmS Code : F-E, S-E
Marine pollutant : yes

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR

UN/ID/NA number : UN 1262
Proper shipping name : Octanes SOLUTION

Class : 3

Packing group : II
Labels : Class 3 - Flammable liquids
ERG Code : 128
Marine pollutant : no
Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
isooctane	540-84-1	1000	1007

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : Fire Hazard
Acute Health Hazard
Chronic Health Hazard

SARA 313

: The following components are subject to reporting levels established by SARA Title III, Section 313:

Bis(2-ethylhexyl) phthalate	117-81-7	>= 0.1 - < 1 %
-----------------------------	----------	----------------

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

The following chemical(s) are listed as HAP under the U.S. Clean Air Act, Section 112 (40 CFR 61):

isooctane	540-84-1	>= 90 - <= 100 %
-----------	----------	------------------

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM Intermediate or Final VOC's (40 CFR 60.489).

Clean Water Act

The following Hazardous Substances are listed under the U.S. CleanWater Act, Section 311, Table 116.4A:

dibutyl phthalate	84-74-2	>= 0.1 - < 1 %
-------------------	---------	----------------

The following Hazardous Chemicals are listed under the U.S. CleanWater Act, Section 311, Table 117.3:

dibutyl phthalate	84-74-2	>= 0.1 - < 1 %
-------------------	---------	----------------

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations**Massachusetts Right To Know**

isooctane	540-84-1
Bis(2-ethylhexyl) phthalate	117-81-7

Pennsylvania Right To Know

isooctane	540-84-1
Benzyl butyl phthalate	85-68-7
Dioctyl phthalate	117-84-0
dibutyl phthalate	84-74-2
Bis(2-ethylhexyl) phthalate	117-81-7
Diethyl phthalate	84-66-2
Dimethyl phthalate	131-11-3
bis(2-ethylhexyl) adipate	103-23-1

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Benzyl butyl phthalate	85-68-7
Dioctyl phthalate	117-84-0
dibutyl phthalate	84-74-2
Bis(2-ethylhexyl) phthalate	117-81-7

Supelco - 40077-U

Page 22 of 24

Diethyl phthalate

84-66-2

Washington Chemicals of High Concern

Benzyl butyl phthalate

85-68-7

Dioctyl phthalate

117-84-0

dibutyl phthalate

84-74-2

Bis(2-ethylhexyl) phthalate

117-81-7

Diethyl phthalate

84-66-2

California Prop. 65

WARNING: This product can expose you to chemicals including Bis(2-ethylhexyl) phthalate, which is/are known to the State of California to cause cancer, and Benzyl butyl phthalate, dibutyl phthalate, Bis(2-ethylhexyl) phthalate, which is/are known to the State of California to cause birth defects or other reproductive harm. For more information go to www.P65Warnings.ca.gov. **The components of this product are reported in the following inventories:**

US TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

ACGIH : USA. ACGIH Threshold Limit Values (TLV)
ACGIH BEI : ACGIH - Biological Exposure Indices (BEI)
NIOSH REL : USA. NIOSH Recommended Exposure Limits
OSHA Z-1 : USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
ACGIH / TWA : 8-hour, time-weighted average
NIOSH REL / TWA : Time-weighted average concentration for up to a 10-hour workday during a 40-hour workweek
NIOSH REL / ST : STEL - 15-minute TWA exposure that should not be exceeded at any time during a workday
OSHA Z-1 / TWA : 8-hour time weighted average

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and

Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2025 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

Revision Date : 07/15/2026

US / EN