SECTION-1: Identification of the substance / mixture and the company / undertaking

Catalogue Number	CS-T-44948
Product Name	Tributyl O-Acetylcitrate
CAS No.	77-90-7
Category	Intermediate
Synonyms	Acetyltributyl Citrate
Brand	Clearsynth Labs Ltd.
Identified uses	Laboratory Chemicals
Uses advised against	Not available
Company	Clearsynth Labs Ltd. Mumbai, India
Emergency Phone #	+91-22-245045900
REACH No.	Not available

SECTION 2: Hazards identification

Disclaimer: This is sample MSDS. Please email **sales@clearsynth.com** for more details.

2.1 Classification of the substance or mixture-Regulation (EC) No 1272/2008:

Not available

2.2 Label Elements

Signal Word: Not available

Not available

Hazard Statement(s)

Code	Statement
Not available	Not available

Precautionary Statement(s)

Code	Statement
Not available	Not available

SECTION 3: Composition / information on ingredients

3.1 Substance

Component : Tributyl O-Acetylcitrate
CAS Number : 77-90-7
Molecular Formula : C20H34O8
Molecular Weight : 402.5
Parent Chemical : Acetyltributyl Citrate
Synonyms : Acetyltributyl Citrate
Concentration : Not available

SECTION 4: First aid measures

SECTION 4: First-aid measures

4.1 Description of first aid measures
- General advice: Remove contaminated clothing and shoes. Seek medical attention if symptoms persist or develop.
- Inhalation: Move person to fresh air. If breathing is difficult, seek medical attention.
- Skin contact: Wash with soap and plenty of water. Get medical attention if irritation occurs.
- Eye contact: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing. Seek medical attention if irritation persists.
- Ingestion: Rinse mouth. Do not induce vomiting unless directed by medical personnel. Seek medical attention if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed
- Not available.

4.3 Indication of any immediate medical attention and special treatment needed
- Treat symptomatically.
- No data available.

SECTION 5: Firefighting measures

SECTION 5: Fire-fighting measures

5.1 Extinguishing media
- Suitable extinguishing media: Water spray, alcohol-resistant foam, dry chemical, carbon dioxide (CO2).
- Unsuitable extinguishing media: Not available.

5.2 Special hazards arising from the substance or mixture
- Combustion may produce carbon oxides.
- Other hazardous decomposition products: Not available.

5.3 Advice for firefighters
- Wear self-contained breathing apparatus (SCBA) and full protective gear.
- Use water spray to cool unopened containers.
- Avoid inhalation of combustion products.

SECTION 6: Accidental release measures

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

- Avoid contact with skin and eyes.
- Provide adequate ventilation.
- Use appropriate personal protective equipment (see Section 8).

6.2 Environmental precautions
- Prevent further leakage or spillage if safe to do so.
- Avoid release to the environment. Do not allow to enter drains/surface waters/groundwater.

6.3 Methods and material for containment and cleaning up
- Contain spill with inert absorbent material (e.g., sand, earth, vermiculite).
- Collect into suitable, labeled containers for disposal.
- Clean contaminated area with water and detergent as appropriate.

6.4 Reference to other sections
- See Section 8 for personal protective equipment.
- See Section 13 for disposal considerations.

SECTION-7: Handling and storage

SECTION 7: Handling and storage

7.1 Precautions for safe handling
- Avoid breathing vapors/mists.
- Avoid contact with skin, eyes, and clothing.
- Use with adequate ventilation.
- Wash thoroughly after handling.

7.2 Conditions for safe storage, including any incompatibilities
- Store in tightly closed container.
- Store in a cool, dry, well-ventilated place.
- Keep away from incompatible materials.
- Incompatible materials: Not available.

7.3 Specific end use(s)
- Intermediate. Specific uses: Not available.

SECTION 8: Exposure controls / personal protection

SECTION 8: Exposure controls/personal protection

8.1 Control parameters
- Occupational exposure limits: Not available.
- Biological limit values: Not available.

8.2 Exposure controls
- Appropriate engineering controls: Use local exhaust ventilation or general ventilation to maintain exposure below applicable limits.

Personal protective equipment (PPE)
- Eye/face protection: Safety glasses with side shields or chemical splash goggles.
- Skin protection: Protective gloves. Select glove material based on permeation and degradation data (not available).
- Body protection: Lab coat or suitable protective clothing.

- Respiratory protection: If ventilation is inadequate, use appropriate respiratory protection. Specific recommendations: Not available.

Hygiene measures
- Handle in accordance with good industrial hygiene and safety practice.
- Wash hands before breaks and at end of workday.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Test	Result
Appearance	No data available
IR spectrum	No data available
pH	No data available
Solubility	No data available

Property	Value
a) Physical State	No data available
b) Color	No data available
c) Odor	No data available
d) pH	No data available
e) Vapour Pressure	No data available
f) Viscosity	No data available
g) Initial Boiling Point and boiling range	No data available
h) Melting Point / Freezing Point	No data available
i) Auto Ignition Temperature	No data available
j) Flash Point	No data available
k) Explosion Limit, Lower	No data available
l) Explosion Limit, Upper	No data available
m) Decomposition Temperature	No data available
n) Loss on Drying	No data available
o) Relative Density	No data available

Property	Value
p) Solubility (in DMSO)	No data available
q) Oxidizing Properties	No data available

SECTION 10: Stability and reactivity

SECTION 10: Stability and reactivity

10.1 Reactivity
- No data available.

10.2 Chemical stability
- Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
- No data available.

10.4 Conditions to avoid
- Heat, flames, and other ignition sources. Other conditions: Not available.

10.5 Incompatible materials
- Not available.

10.6 Hazardous decomposition products
- Carbon oxides. Other decomposition products: Not available.

SECTION 11: Toxicological information

11.1 Information on toxicological effects
- Acute toxicity: IDENTIFICATION AND USE: Acetyl tributyl citrate (ATBC) is a colorless liquid. It is the most widely used phthalate substitute plasticizer. It is used in products such as food wrap, vinyl toys, and pharmaceutical excipients. It is also used as a flavor ingredient in non-alcoholic beverages. HUMAN EXPOSURE AND TOXICITY: The skin irritation potential of acetyl tributyl citrate was evaluated using 59 men and women, all of whom had history of diabetes, psoriasis, or active dermatoses. ATBC was nonirritating to the skin, and reactions suggestive of contact sensitization were not observed during the study. In vitro ATBC increased CYP3A4 messenger RNA (mRNA) levels and enzyme activity in the human intestinal cells but not in human liver cells. ANIMAL STUDIES: Acute oral toxicity of ATBC in cats and rats is low. CYP3A1 mRNA levels were increased in the intestine but not the liver of ATBC-treated rats. In a 90-day repeated-dose oral dietary study in rats, decreased body weight and organ weight changes were observed at 1000 mg/kg-bw/day. In a combined repeated dose/reproductive/developmental toxicity study in rats, organ weight and histopathological changes were observed in adults at 1000 mg/kg-bw/day. In a 2-generation reproductive toxicity study in rats, reduced body weight was observed in F1 males at 300 mg/kg-bw/day. In the same study, no other treatment related effects were observed. In the combined repeated dose/reproductive/developmental toxicity study in rats previously described, histopathological changes were observed in the liver of adult males at 300 mg/kg-bw/day. In the same study, decreased litter size and decreased number of implantations were observed at 1000 mg/kg-bw/day. ATBC did not induce gene mutations in bacteria or mammalian cells in vitro and did not induce chromosomal aberrations in mammalian cells in vitro. ECOTOXICITY STUDIES: For acetyl tributyl citrate, the 96-hr LC50 values for fish range from 38 to 60 mg/L, the 48-hr EC50 value for aquatic invertebrates is 7.8 mg/L and the 72-hr EC50 values for aquatic plants are 11.5 mg/L for biomass and 74.4mg/L for growth rate, respectively. /ALTERNATIVE and IN VITRO TESTS/ The cytotoxicity of

acetyl-tributyl-citrate and dibutyl-sebacate was studied in cultured mammalian cells. The impetus for the study was a report that acetyl-tributyl-citrate and dibutyl-sebacate, which were plasticizers found in polyvinylidene-chloride film used for packaging food, could leach out and diffuse into the foods. Human KB cells, monkey Vero cells, and canine MDCK cells were incubated with acetyl-tributyl-citrate or dibutyl sebacate over a range of concentrations for 72 hours. Cytotoxicity was evaluated by determining the extent of growth inhibition. Doses of acetyl-tributyl-citrate and dibutyl-sebacate that inhibited growth by 50% were calculated from the data. Both compounds inhibited the growth of all cells in a dose dependent manner. The inhibited growth by 50% of acetyl-tributyl-citrate in the various types were: 44.7 ug/mL in KB cells; 39.9 ug/mL in Vero cells; and 42.1 ug/mL in MDCK cells. The inhibited growth by 50% of dibutyl-sebacate in these cells were: KB cells, 1,549 ug/mL; Vero cells, 1,510 ug/mL; and MDCK cells, 1,549 ug/mL. /It was/ concluded that when comparing the results of this study with those obtained previously using tricresyl-phosphate,triphenyl-phosphate (TPP), butylated-hydroxyanisole, and butylated-hydroxytoluene in human KB cells, acetyl-tributyl-citrate is more toxic than TCP and more toxic than TPP. Acetyl-tributyl-citrate is less toxic than BHA, but shows toxicity similar to that of BHT. DBS is much less toxic than either BHT or BHA. KB, Vero, and MDCK cells show similar sensitivity to acetyl-tributyl-citrate and DBS.
- Skin corrosion/irritation: IDENTIFICATION AND USE: Acetyl tributyl citrate (ATBC) is a colorless liquid. It is the most widely used phthalate substitute plasticizer. It is used in products such as food wrap, vinyl toys, and pharmaceutical excipients. It is also used as a flavor ingredient in non-alcoholic beverages. HUMAN EXPOSURE AND TOXICITY: The skin irritation potential of acetyl tributyl citrate was evaluated using 59 men and women, all of whom had history of diabetes, psoriasis, or active dermatoses. ATBC was nonirritating to the skin, and reactions suggestive of contact sensitization were not observed during the study. In vitro ATBC increased CYP3A4 messenger RNA (mRNA) levels and enzyme activity in the human intestinal cells but not in human liver cells. ANIMAL STUDIES: Acute oral toxicity of ATBC in cats and rats is low. CYP3A1 mRNA levels were increased in the intestine but not the liver of ATBC-treated rats. In a 90-day repeated-dose oral dietary study in rats, decreased body weight and organ weight changes were observed at 1000 mg/kg-bw/day. In a combined repeated dose/reproductive/developmental toxicity study in rats, organ weight and histopathological changes were observed in adults at 1000 mg/kg-bw/day. In a 2-generation reproductive toxicity study in rats, reduced body weight was observed in F1 males at 300 mg/kg-bw/day. In the same study, no other treatment related effects were observed. In the combined repeated dose/reproductive/developmental toxicity study in rats previously described, histopathological changes were observed in the liver of adult males at 300 mg/kg-bw/day. In the same study, decreased litter size and decreased number of implantations were observed at 1000 mg/kg-bw/day. ATBC did not induce gene mutations in bacteria or mammalian cells in vitro and did not induce chromosomal aberrations in mammalian cells in vitro. ECOTOXICITY STUDIES: For acetyl tributyl citrate, the 96-hr LC50 values for fish range from 38 to 60 mg/L, the 48-hr EC50 value for aquatic invertebrates is 7.8 mg/L and the 72-hr EC50 values for aquatic plants are 11.5 mg/L for biomass and 74.4mg/L for growth rate, respectively. /HUMAN EXPOSURE STUDIES/ The skin irritation potential of acetyl tributyl citrate was evaluated using 59 men and women (age range = 21-60 years), all of whom had history of diabetes, psoriasis, or active dermatoses. ... Occlusive patches moistened with 0.4 mL of acetyl tributyl citrate were applied to the upper arm of each subject on Mondays, Wednesdays, and Fridays for 3 consecutive weeks. Each patch was removed 24 hours post application. Induction reactions were scored prior to patch applications (second through ninth visits) and at the time of the tenth visit. Duplicate challenge of the test material was made after a two-week non-treatment period. ... One challenge patch was applied to the original test site, and , another, to an adjacent site. Challenge reactions were scored at 48 and 96 hours post application. /Acetyl tributyl citrate/ was nonirritating to the skin, and reactions suggestive of contact sensitization were not observed during the study.
- Serious eye damage/eye irritation: No data available.
- Respiratory or skin sensitization: IDENTIFICATION AND USE: Acetyl tributyl citrate (ATBC) is a colorless liquid. It is the most widely used phthalate substitute plasticizer. It is used in products such as food wrap, vinyl toys, and

pharmaceutical excipients. It is also used as a flavor ingredient in non-alcoholic beverages. HUMAN EXPOSURE AND TOXICITY: The skin irritation potential of acetyl tributyl citrate was evaluated using 59 men and women, all of whom had history of diabetes, psoriasis, or active dermatoses. ATBC was nonirritating to the skin, and reactions suggestive of contact sensitization were not observed during the study. In vitro ATBC increased CYP3A4 messenger RNA (mRNA) levels and enzyme activity in the human intestinal cells but not in human liver cells. ANIMAL STUDIES: Acute oral toxicity of ATBC in cats and rats is low. CYP3A1 mRNA levels were increased in the intestine but not the liver of ATBC-treated rats. In a 90-day repeated-dose oral dietary study in rats, decreased body weight and organ weight changes were observed at 1000 mg/kg-bw/day. In a combined repeated dose/reproductive/developmental toxicity study in rats, organ weight and histopathological changes were observed in adults at 1000 mg/kg-bw/day. In a 2-generation reproductive toxicity study in rats, reduced body weight was observed in F1 males at 300 mg/kg-bw/day. In the same study, no other treatment related effects were observed. In the combined repeated dose/reproductive/developmental toxicity study in rats previously described, histopathological changes were observed in the liver of adult males at 300 mg/kg-bw/day. In the same study, decreased litter size and decreased number of implantations were observed at 1000 mg/kg-bw/day. ATBC did not induce gene mutations in bacteria or mammalian cells in vitro and did not induce chromosomal aberrations in mammalian cells in vitro. ECOTOXICITY STUDIES: For acetyl tributyl citrate, the 96-hr LC50 values for fish range from 38 to 60 mg/L, the 48-hr EC50 value for aquatic invertebrates is 7.8 mg/L and the 72-hr EC50 values for aquatic plants are 11.5 mg/L for biomass and 74.4mg/L for growth rate, respectively. /HUMAN EXPOSURE STUDIES/ The skin irritation potential of acetyl tributyl citrate was evaluated using 59 men and women (age range = 21-60 years), all of whom had history of diabetes, psoriasis, or active dermatoses. ... Occlusive patches moistened with 0.4 mL of acetyl tributyl citrate were applied to the upper arm of each subject on Mondays, Wednesdays, and Fridays for 3 consecutive weeks. Each patch was removed 24 hours post application. Induction reactions were scored prior to patch applications (second through ninth visits) and at the time of the tenth visit. Duplicate challenge of the test material was made after a two-week non-treatment period. ... One challenge patch was applied to the original test site, and , another, to an adjacent site. Challenge reactions were scored at 48 and 96 hours post application. /Acetyl tributyl citrate/ was nonirritating to the skin, and reactions suggestive of contact sensitization were not observed during the study.

- Germ cell mutagenicity: IDENTIFICATION AND USE: Acetyl tributyl citrate (ATBC) is a colorless liquid. It is the most widely used phthalate substitute plasticizer. It is used in products such as food wrap, vinyl toys, and pharmaceutical excipients. It is also used as a flavor ingredient in non-alcoholic beverages. HUMAN EXPOSURE AND TOXICITY: The skin irritation potential of acetyl tributyl citrate was evaluated using 59 men and women, all of whom had history of diabetes, psoriasis, or active dermatoses. ATBC was nonirritating to the skin, and reactions suggestive of contact sensitization were not observed during the study. In vitro ATBC increased CYP3A4 messenger RNA (mRNA) levels and enzyme activity in the human intestinal cells but not in human liver cells. ANIMAL STUDIES: Acute oral toxicity of ATBC in cats and rats is low. CYP3A1 mRNA levels were increased in the intestine but not the liver of ATBC-treated rats. In a 90-day repeated-dose oral dietary study in rats, decreased body weight and organ weight changes were observed at 1000 mg/kg-bw/day. In a combined repeated dose/reproductive/developmental toxicity study in rats, organ weight and histopathological changes were observed in adults at 1000 mg/kg-bw/day. In a 2-generation reproductive toxicity study in rats, reduced body weight was observed in F1 males at 300 mg/kg-bw/day. In the same study, no other treatment related effects were observed. In the combined repeated dose/reproductive/developmental toxicity study in rats previously described, histopathological changes were observed in the liver of adult males at 300 mg/kg-bw/day. In the same study, decreased litter size and decreased number of implantations were observed at 1000 mg/kg-bw/day. ATBC did not induce gene mutations in bacteria or mammalian cells in vitro and did not induce chromosomal aberrations in mammalian cells in vitro. ECOTOXICITY STUDIES: For acetyl tributyl citrate, the 96-hr LC50 values for fish range from 38 to 60 mg/L, the 48-hr EC50 value for aquatic invertebrates is 7.8 mg/L and the 72-hr EC50 values for

aquatic plants are 11.5 mg/L for biomass and 74.4mg/L for growth rate, respectively.
- Carcinogenicity: No data available.
- Reproductive toxicity: IDENTIFICATION AND USE: Acetyl tributyl citrate (ATBC) is a colorless liquid. It is the most widely used phthalate substitute plasticizer. It is used in products such as food wrap, vinyl toys, and pharmaceutical excipients. It is also used as a flavor ingredient in non-alcoholic beverages. HUMAN EXPOSURE AND TOXICITY: The skin irritation potential of acetyl tributyl citrate was evaluated using 59 men and women, all of whom had history of diabetes, psoriasis, or active dermatoses. ATBC was nonirritating to the skin, and reactions suggestive of contact sensitization were not observed during the study. In vitro ATBC increased CYP3A4 messenger RNA (mRNA) levels and enzyme activity in the human intestinal cells but not in human liver cells. ANIMAL STUDIES: Acute oral toxicity of ATBC in cats and rats is low. CYP3A1 mRNA levels were increased in the intestine but not the liver of ATBC-treated rats. In a 90-day repeated-dose oral dietary study in rats, decreased body weight and organ weight changes were observed at 1000 mg/kg-bw/day. In a combined repeated dose/reproductive/developmental toxicity study in rats, organ weight and histopathological changes were observed in adults at 1000 mg/kg-bw/day. In a 2-generation reproductive toxicity study in rats, reduced body weight was observed in F1 males at 300 mg/kg-bw/day. In the same study, no other treatment related effects were observed. In the combined repeated dose/reproductive/developmental toxicity study in rats previously described, histopathological changes were observed in the liver of adult males at 300 mg/kg-bw/day. In the same study, decreased litter size and decreased number of implantations were observed at 1000 mg/kg-bw/day. ATBC did not induce gene mutations in bacteria or mammalian cells in vitro and did not induce chromosomal aberrations in mammalian cells in vitro. ECOTOXICITY STUDIES: For acetyl tributyl citrate, the 96-hr LC50 values for fish range from 38 to 60 mg/L, the 48-hr EC50 value for aquatic invertebrates is 7.8 mg/L and the 72-hr EC50 values for aquatic plants are 11.5 mg/L for biomass and 74.4mg/L for growth rate, respectively.
- STOT-single exposure: No data available.
- STOT-repeated exposure: No data available.
- Aspiration hazard: No data available.

Likely routes of exposure
- No data available.

Symptoms related to the physical, chemical and toxicological characteristics
- IDENTIFICATION AND USE: Acetyl tributyl citrate (ATBC) is a colorless liquid. It is the most widely used phthalate substitute plasticizer. It is used in products such as food wrap, vinyl toys, and pharmaceutical excipients. It is also used as a flavor ingredient in non-alcoholic beverages. HUMAN EXPOSURE AND TOXICITY: The skin irritation potential of acetyl tributyl citrate was evaluated using 59 men and women, all of whom had history of diabetes, psoriasis, or active dermatoses. ATBC was nonirritating to the skin, and reactions suggestive of contact sensitization were not observed during the study. In vitro ATBC increased CYP3A4 messenger RNA (mRNA) levels and enzyme activity in the human intestinal cells but not in human liver cells. ANIMAL STUDIES: Acute oral toxicity of ATBC in cats and rats is low. CYP3A1 mRNA levels were increased in the intestine but not the liver of ATBC-treated rats. In a 90-day repeated-dose oral dietary study in rats, decreased body weight and organ weight changes were observed at 1000 mg/kg-bw/day. In a combined repeated dose/reproductive/developmental toxicity study in rats, organ weight and histopathological changes were observed in adults at 1000 mg/kg-bw/day. In a 2-generation reproductive toxicity study in rats, reduced body weight was observed in F1 males at 300 mg/kg-bw/day. In the same study, no other treatment related effects were observed. In the combined repeated dose/reproductive/developmental toxicity study in rats previously described, histopathological changes were observed in the liver of adult males at 300 mg/kg-bw/day. In the same study, decreased litter size and decreased number of implantations were observed at 1000 mg/kg-bw/day. ATBC did not induce gene mutations in bacteria or mammalian cells in vitro and did not induce chromosomal aberrations in mammalian cells in vitro. ECOTOXICITY STUDIES: For acetyl tributyl citrate, the 96-hr

LC50 values for fish range from 38 to 60 mg/L, the 48-hr EC50 value for aquatic invertebrates is 7.8 mg/L and the 72-hr EC50 values for aquatic plants are 11.5 mg/L for biomass and 74.4mg/L for growth rate, respectively.

SECTION 12: Ecological information

SECTION 12: Ecological information

12.1 Toxicity
- No data available.

12.2 Persistence and degradability
- No data available.

12.3 Bioaccumulative potential
- No data available.

12.4 Mobility in soil
- No data available.

12.5 Results of PBT and vPvB assessment
- Not available.

12.6 Endocrine disrupting properties
- Not available.

12.7 Other adverse effects
- No data available.

SECTION 13: Disposal considerations

SECTION 13: Disposal considerations

13.1 Waste treatment methods
- Dispose of contents/container in accordance with local/regional/national/international regulations.
- Do not discharge to drains or the environment.
- Waste treatment options: Not available.
- Contaminated packaging: Dispose of as unused product unless cleaned appropriately.

SECTION 14: Transport information

SECTION 14: Transport information

- UN number: Not available.
- UN proper shipping name: Not available.
- Transport hazard class(es): Not available.
- Packing group: Not available.
- Environmental hazards: Not available.
- Special precautions for user: Not available.
- Transport in bulk according to IMO instruments: Not available.

Additional information

- Classification for transport (ADR/RID, IMDG, IATA): Not available.

SECTION 15: Regulatory information

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture
- Regulatory listings (e.g., TSCA, REACH, DSL, AICS, ENCS, IECSC, KECI, PICCS): Not available.

15.2 Chemical safety assessment
- No data available.

SECTION 16: Other information

SECTION 16: Other information

- Product name: Tributyl O-Acetylcitrate
- Synonyms: Acetyltributyl Citrate
- CAS No.: 77-90-7
- Catalog No.: CS-T-44948
- Supplier: Clearsynth Labs Ltd., Mumbai, India
- Emergency phone: +91-22-245045900

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- The information provided is believed to be accurate based on available data, but no warranty is expressed or implied. Users should determine suitability for their particular purpose and comply with all applicable regulations.

Revision information
- Revision date: Not available.
- Version: Not available.

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