

MATERIAL SAFETY DATA SHEET

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Version 1.6

Section 1 - Product and Company Information

Product Name 4-ISOBUTYL-ALPHA-METHYLPHENYLACETIC
ACID , 99%

Product Number 284742

Brand ALDRICH

Company Sigma-Aldrich

Address 3050 Spruce Street
SAINT LOUIS MO 63103 US

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Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313
4-ISOBUTYL-ALPHA-METHYLPHENYLACETIC ACID	15687-27-1	No

Formula C13H18O2

Synonyms Acide (isobutyl-4 phenyl)-2 propionique (French)
* Adran * Advil * Anflagen * Artril 300 *
Benzeneacetic acid,
alpha-methyl-4-(2-methylpropyl)- * Bluton *
Brufanic * Brufen * Buburone * Butylenin * Dolgin
* Epobron * Ibufen * Ibuprocin * Ibuprofen *
IP-82 * p-Isobutylhydratropic acid *
4-Isobutylhydratropic acid *
2-(4-Isobutylphenyl)propanoic acid *
alpha-p-Isobutylphenylpropionic acid *
alpha-(4-Isobutylphenyl)propionic acid *
2-(p-Isobutylphenyl)propionic acid * Lamidon *
Liptan * Motrin * Mynosedin * Napacetin *
Nobfelon * Nobfen * Nobgen * Nuprin * Nurofen *
Paduden * Proflex * RD 13621 * Rebugen * Roidenin
* Rufin * Unipron

RTECS Number: MU6640000

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Harmful.
Harmful if swallowed.
Target organ(s): Kidneys.

HMIS RATING

HEALTH: 1*
FLAMMABILITY: 0
REACTIVITY: 0

NFPA RATING

HEALTH: 1

FLAMMABILITY: 0

REACTIVITY: 0

*additional chronic hazards present.

For additional information on toxicity, please refer to Section 11.

Section 4 - First Aid Measures

ORAL EXPOSURE

If swallowed, wash out mouth with water provided person is conscious. Call a physician.

INHALATION EXPOSURE

If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

DERMAL EXPOSURE

In case of skin contact, flush with copious amounts of water for at least 15 minutes. Remove contaminated clothing and shoes. Call a physician.

EYE EXPOSURE

In case of contact with eyes, flush with copious amounts of water for at least 15 minutes. Assure adequate flushing by separating the eyelids with fingers. Call a physician.

Section 5 - Fire Fighting Measures

FLASH POINT

N/A

AUTOIGNITION TEMP

N/A

FLAMMABILITY

N/A

FIREFIGHTING

Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.
Specific Hazard(s): Emits toxic fumes under fire conditions.

Section 6 - Accidental Release Measures

PROCEDURE TO BE FOLLOWED IN CASE OF LEAK OR SPILL

Evacuate area.

PROCEDURE(S) OF PERSONAL PRECAUTION(S)

Wear self-contained breathing apparatus, rubber boots, and heavy rubber gloves.

METHODS FOR CLEANING UP

Sweep up, place in a bag and hold for waste disposal. Avoid raising dust. Ventilate area and wash spill site after material pickup is complete.

Section 7 - Handling and Storage

HANDLING

User Exposure: Do not breathe dust. Avoid contact with eyes, skin, and clothing. Avoid prolonged or repeated exposure.

STORAGE

Suitable: Keep tightly closed.

Section 8 - Exposure Controls / PPE

ENGINEERING CONTROLS

Safety shower and eye bath. Mechanical exhaust required.

PERSONAL PROTECTIVE EQUIPMENT

Respiratory: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). Where risk assessment shows air-purifying respirators are appropriate use a dust mask type N95 (US) or type P1 (EN 143) respirator.

Hand: Compatible chemical-resistant gloves.

Eye: Chemical safety goggles.

GENERAL HYGIENE MEASURES

Wash thoroughly after handling.

Section 9 - Physical/Chemical Properties

Appearance	Physical State: Solid	
Property	Value	At Temperature or Pressure
Molecular Weight	206.29 AMU	
pH	N/A	
BP/BP Range	N/A	
MP/MP Range	77.0 - 78.0 °C	
Freezing Point	N/A	
Vapor Pressure	N/A	
Vapor Density	N/A	
Saturated Vapor Conc.	N/A	
SG/Density	N/A	
Bulk Density	N/A	
Odor Threshold	N/A	
Volatile%	N/A	
VOC Content	N/A	
Water Content	N/A	
Solvent Content	N/A	
Evaporation Rate	N/A	
Viscosity	N/A	
Surface Tension	N/A	
Partition Coefficient	N/A	
Decomposition Temp.	N/A	
Flash Point	N/A	
Explosion Limits	N/A	
Flammability	N/A	
Autoignition Temp	N/A	
Refractive Index	N/A	
Optical Rotation	N/A	
Miscellaneous Data	N/A	
Solubility	N/A	

N/A = not available

Section 10 - Stability and Reactivity

STABILITY

Stable: Stable.

Materials to Avoid: Strong oxidizing agents.

HAZARDOUS DECOMPOSITION PRODUCTS

Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide.

HAZARDOUS POLYMERIZATION

Hazardous Polymerization: Will not occur

Section 11 - Toxicological Information

ROUTE OF EXPOSURE

Skin Contact: May cause skin irritation.

Skin Absorption: May be harmful if absorbed through the skin.

Eye Contact: May cause eye irritation.

Inhalation: Material may be irritating to mucous membranes and upper respiratory tract. May be harmful if inhaled.

Ingestion: Harmful if swallowed.

SENSITIZATION

Sensitization: Prolonged or repeated exposure may cause allergic reactions in certain sensitive individuals.

TARGET ORGAN(S) OR SYSTEM(S)

Kidneys.

SIGNS AND SYMPTOMS OF EXPOSURE

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. Clinical trials have shown the following possible adverse reactions: gastrointestinal disturbances including nausea, vomiting, cramps, diarrhea, constipation, bloating, central nervous system effects which include dizziness, headache, depression, insomnia, aseptic meningitis, somnolence, dermatological effects of maculopapular and vesiculobullous eruptions, urticaria, alopecia, erythema multiforme, stevens-johnson syndrome, hematologic effects of neutropenia, aplastic and hemolytic anemia, thrombocytopenia, decreases in hemoglobin and hematocrit.

TOXICITY DATA

Oral

Man

171 mg/kg

LDLO

Remarks: Behavioral:General anesthetic. Vascular:BP lowering not characterized in autonomic section.

Oral

Child

469 mg/kg

LDLO

Remarks: Behavioral:Convulsions or effect on seizure threshold. Lungs, Thorax, or Respiration:Dyspnea.

Oral

Rat

636 mg/kg

LD50

Intraperitoneal

Rat

626 MG/KG

LD50

Remarks: Biochemical:Metabolism (intermediary): Effect on inflammation or mediation of inflammation. Nutritional and Gross Metabolic:Changes in:Body temperature decrease.
Behavioral:Analgesia.

Subcutaneous

Rat

740 MG/KG

LD50

Rectal

Rat

530 MG/KG

LD50

Remarks: Behavioral:Altered sleep time (including change in righting reflex). Behavioral:Change in motor activity (specific assay). Gastrointestinal:Hypermotility, diarrhea.

Oral

Mouse

740 mg/kg

LD50

Remarks: Behavioral:Analgesia.

Intraperitoneal

Mouse

320 MG/KG

LD50

Remarks: Behavioral:Altered sleep time (including change in righting reflex). Gastrointestinal:Ulceration or bleeding from stomach.

Subcutaneous

Mouse

395 MG/KG

LD50

Rectal

Mouse

620 MG/KG

LD50

Remarks: Gastrointestinal:Hypermotility, diarrhea.
Behavioral:Change in motor activity (specific assay).
Behavioral:Altered sleep time (including change in righting reflex).

Oral

Rabbit

1400 mg/kg

LD50

Rectal

Rabbit

830 MG/KG

LD50

Oral

Guinea pig

495 mg/kg

LD50

Oral
Hamster
1690 mg/kg
LD50

Oral
Mammal
1000 mg/kg
LD50

CHRONIC EXPOSURE - TERATOGEN

Result: Laboratory experiments have shown teratogenic effects.

Species: Rat
Dose: 840 MG/KG
Route of Application: Oral
Exposure Time: (8-14D PREG)
Result: Effects on Newborn: Growth statistics (e.g., reduced weight gain). Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).

Species: Rat
Dose: 10 MG/KG
Route of Application: Oral
Exposure Time: (21D PREG)
Result: Effects on Embryo or Fetus: Other effects to embryo.

Species: Rat
Dose: 810 MG/KG
Route of Application: Rectal
Exposure Time: (60D MALE/2W PRE-7D PREG)
Result: Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).

Species: Mouse
Dose: 1260 MG/KG
Route of Application: Oral
Exposure Time: (7-13D PREG)
Result: Effects on Embryo or Fetus: Fetal death. Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).

CHRONIC EXPOSURE - MUTAGEN

Species: Mouse
Route: Oral
Dose: 1470 MG/KG
Exposure Time: 7D
Mutation test: Cytogenetic analysis

Species: Mouse
Route: Intraperitoneal
Dose: 50 MG/KG
Mutation test: Sister chromatid exchange

Species: Mouse
Route: Oral
Dose: 270 MG/KG
Mutation test: Sister chromatid exchange

CHRONIC EXPOSURE - REPRODUCTIVE HAZARD

Species: Woman
Dose: 8 MG/KG
Route of Application: Oral
Exposure Time: (1D PRE)
Result: Maternal Effects: Menstrual cycle changes or disorders.

Species: Rat
Dose: 600 MG/KG
Route of Application: Oral
Exposure Time: (3-5D PREG)
Result: Effects on Fertility: Litter size (e.g.; # fetuses per litter; measured before birth). Effects on Fertility: Pre-implantation mortality (e.g., reduction in number of implants per female; total number of implants per corpora lutea).

Species: Rat
Dose: 9750 MG/KG
Route of Application: Oral
Exposure Time: (65D MALE)
Result: Paternal Effects: Spermatogenesis (including genetic material, sperm morphology, motility, and count). Paternal Effects: Testes, epididymis, sperm duct.

Species: Rat
Dose: 2 MG/KG
Route of Application: Intrauterine
Exposure Time: (4D PREG)
Result: Effects on Fertility: Pre-implantation mortality (e.g., reduction in number of implants per female; total number of implants per corpora lutea).

Species: Rat
Dose: 270 MG/KG
Route of Application: Rectal
Exposure Time: (17-21D PREG)
Result: Effects on Newborn: Live birth index (# fetuses per litter; measured after birth). Maternal Effects: Parturition.

Species: Rat
Dose: 891 MG/KG
Route of Application: Rectal
Exposure Time: (17-21D PREG/21D POST)
Result: Effects on Newborn: Weaning or lactation index (e.g., # alive at weaning per # alive at day 4).

Species: Rat
Dose: 1 GM/KG
Route of Application: Rectal
Exposure Time: (17-21D PREG/4D POST)
Result: Effects on Newborn: Viability index (e.g., # alive at day 4 per # born alive).

Species: Rat
Dose: 8100 MG/KG
Route of Application: Rectal
Exposure Time: (60D MALE/2W PRE-7D PREG)
Result: Effects on Fertility: Pre-implantation mortality (e.g., reduction in number of implants per female; total number of implants per corpora lutea). Effects on Fertility: Litter size (e.g.; # fetuses per litter; measured before birth).

Species: Mouse
Dose: 420 MG/KG
Route of Application: Oral
Exposure Time: (7-13D PREG)
Result: Effects on Fertility: Litter size (e.g.; # fetuses per litter; measured before birth). Effects on Fertility: Pre-implantation mortality (e.g., reduction in number of implants per female; total number of implants per corpora lutea).

Section 12 - Ecological Information

No data available.

Section 13 - Disposal Considerations

APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations.

Section 14 - Transport Information

DOT

Proper Shipping Name: None
Non-Hazardous for Transport: This substance is considered to be non-hazardous for transport.

IATA

Non-Hazardous for Air Transport: Non-hazardous for air transport.

Section 15 - Regulatory Information

EU ADDITIONAL CLASSIFICATION

Symbol of Danger: Xn
Indication of Danger: Harmful.
R: 22
Risk Statements: Harmful if swallowed.
S: 36
Safety Statements: Wear suitable protective clothing.

US CLASSIFICATION AND LABEL TEXT

Indication of Danger: Harmful.
Risk Statements: Harmful if swallowed.
Safety Statements: Wear suitable protective clothing.
US Statements: Target organ(s): Kidneys.

UNITED STATES REGULATORY INFORMATION

SARA LISTED: No
TSCA INVENTORY ITEM: Yes

CANADA REGULATORY INFORMATION

WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.
DSL: Yes
NDSL: No

Section 16 - Other Information

DISCLAIMER

For R&D use only. Not for drug, household or other uses.

WARRANTY

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale. Copyright 2008 Sigma-Aldrich Co. License granted to make unlimited paper copies for internal use only.