



SAFETY DATA SHEET

1. Identification

Product identifier	Ibuprofen Related Compound C
Other means of identification	
Catalog number	1335541
CAS number	38861-78-8
Synonyms	1-[4-(2-Methylpropyl)phenyl]ethan-1-one
Chemical name	4-Isobutylacetophenone
Recommended use	For analytical laboratory use only.
Recommended restrictions	Not for use as a drug. Not for administration to humans or animals.

Manufacturer/Importer/Supplier/Distributor information

Manufacturer

Company name	U. S. Pharmacopeia
Address	12601 Twinbrook Parkway Rockville MD 20852-1790 United States
Telephone	Technical Services 301-816-8129
Website	www.usp.org
E-mail	RSTECH@usp.org
Emergency phone number	CHEMTREC within US & 1-800-424-9300 Canada CHEMTREC outside US & +1 703-527-3887 Canada

2. Hazard(s) identification

Physical hazards	Flammable liquids	Category 3
Health hazards	Serious eye damage/eye irritation	Category 2B
	Sensitization, skin	Category 1
Environmental hazards	Not classified.	
OSHA defined hazards	Not classified.	

Label elements



Signal word	Warning
Hazard statement	Flammable liquid and vapor. May cause an allergic skin reaction. Causes eye irritation.
Precautionary statement	
Prevention	Keep away from heat/sparks/open flames/hot surfaces. Use explosion-proof electrical/ventilating/lighting equipment. Keep container tightly closed. Use only non-sparking tools. Take precautionary measures against static discharge. Avoid breathing mist or vapor. Wash thoroughly after handling. Wear protective gloves/eye protection/face protection. Contaminated work clothing must not be allowed out of the workplace.
Response	If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower. If skin irritation or rash occurs: Get medical advice/attention. Wash contaminated clothing before reuse. If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention. In case of fire: Use appropriate media to extinguish.
Storage	Store in a well-ventilated place. Keep cool.
Disposal	Dispose of contents/container in accordance with local/regional/national/international regulations.

Hazard(s) not otherwise classified (HNOC)	None known.
Supplemental information	Pharmaceutical related compound of unknown potency.

3. Composition/information on ingredients

Substance

Chemical name	Common name and synonyms	CAS number	%
Ibuprofen Related Compound C	1-[4-(2-Methylpropyl)phenyl]ethan-1-one	38861-78-8	100

4. First-aid measures

Inhalation	Move to fresh air. Call a physician if symptoms develop or persist.
Skin contact	Remove contaminated clothing immediately and wash skin with soap and water. In case of eczema or other skin disorders: Seek medical attention and take along these instructions.
Eye contact	Immediately flush eyes with plenty of water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical attention if irritation develops and persists.
Ingestion	Rinse mouth. Get medical attention if symptoms occur.
Most important symptoms/effects, acute and delayed	Pharmaceutical related compound of unknown potency. It is not known if occupational exposure may cause physiological effects.
Indication of immediate medical attention and special treatment needed	Provide general supportive measures and treat symptomatically.
General information	Remove from exposure. Remove contaminated clothing. For treatment advice, seek guidance from an occupational health physician or other licensed health-care provider familiar with workplace chemical exposures. In the United States, the national poison control center phone number is 1-800-222-1222. If person is not breathing, give artificial respiration. If breathing is difficult, give oxygen if available. Persons developing serious hypersensitivity (anaphylactic) reactions must receive immediate medical attention.

5. Fire-fighting measures

Suitable extinguishing media	Water fog. Foam. Dry chemical powder. Carbon dioxide (CO2).
Unsuitable extinguishing media	Do not use water jet as an extinguisher, as this will spread the fire.
Specific hazards arising from the chemical	By heating and fire, harmful vapors/gases may be formed.
Special protective equipment and precautions for firefighters	Wear suitable protective equipment.
Fire fighting equipment/instructions	As with all fires, evacuate personnel to a safe area. Firefighters should use self-contained breathing equipment and protective clothing. Use water spray to cool unopened containers.
Specific methods	Use standard firefighting procedures and consider the hazards of other involved materials.
General fire hazards	Flammable liquid and vapor.

6. Accidental release measures

Personal precautions, protective equipment and emergency procedures	Keep unnecessary personnel away. ELIMINATE all ignition sources (no smoking, flares, sparks or flames in immediate area). Wear appropriate personal protective equipment. Avoid inhalation of vapors. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Ensure adequate ventilation. For personal protection, see section 8 of the SDS.
Methods and materials for containment and cleaning up	Absorb spillage with suitable absorbent material. Remove sources of ignition. Keep combustibles (wood, paper, oil, etc.) away from spilled material. Clean surface thoroughly to remove residual contamination. For waste disposal, see section 13 of the SDS.
Environmental precautions	Avoid discharge into drains, water courses or onto the ground.

7. Handling and storage

Precautions for safe handling	As a general rule, when handling USP materials, avoid all contact and inhalation of dust, mists, and/or vapors associated with the material. Clean equipment and work surfaces with suitable detergent or solvent after use. After removing gloves, wash hands and other exposed skin thoroughly. Select and use containment devices and personal protective equipment based on a risk assessment of material potency and exposure potential.
Conditions for safe storage, including any incompatibilities	Store in tight container. This material should be handled and stored per label instructions to ensure product integrity.

8. Exposure controls/personal protection

Occupational exposure limits

The following constituents are the only constituents of the product which have a PEL, TLV or other recommended exposure limit. At this time, the other constituents have no known exposure limits.

Exposure limit values

Industrial Use Material

Type

Value

Ibuprofen Related
Compound C (CAS
38861-78-8)

STEL

200 mg/m3

Biological limit values

No biological exposure limits noted for the ingredient(s).

Appropriate engineering controls

No open handling. For laboratory operation, use an engineered local exhaust ventilation (LEV) and/or enclosure or isolator system for procedures where aerosolization of solutions may occur (e.g., vortexing, pipetting, pumping). Control the potential for spills and leaks by securing all connections. Control exposures to below the occupational exposure level (if available). Select and use containment devices and personal protective equipment based on a risk assessment of exposure potential. Cover all containers for solutions and slurries while being transferred.

Individual protection measures, such as personal protective equipment

Eye/face protection

Wear safety glasses with side shields, chemical splash goggles, or full face shield, if necessary. Base the choice of protection on the job activity and potential for contact with eyes or face. An emergency eye wash station should be available.

Skin protection

Hand protection

Consider double gloves. Wear nitrile or other impervious gloves if skin contact is possible. When the material is dissolved or suspended in an organic solvent, wear gloves that provide protection against the solvent.

Other

Train employees in proper gowning and degowning practices. Wear disposable lab coat, disposable sleeve covers and two pair of gloves as appropriate for the task. Base the choice of skin protection on the job activity, potential for skin contact and solvents and reagents in use. Do not wear protective garments in common areas (e.g., cafeterias) or out-of-doors.

Respiratory protection

Use a powered air-purifying respirator (PAPR) with HEPA filters, disposable outerware and head cover for spill cleanup. Choose respiratory protection appropriate to the task and the level of existing engineering controls.

Thermal hazards

Wear appropriate thermal protective clothing, when necessary.

General hygiene considerations

Pharmacological effects may be seen with occupational exposure. Handling practices in this SDS are recommendations for laboratory use of USP materials.

9. Physical and chemical properties

Appearance

Appearance descriptions are general information and not specific to any USP lot.

Physical state

Liquid.

Form

Liquid.

Color

Clear. Colourless to light yellow.

Odor

Not available.

Odor threshold

Not available.

pH

Not available.

Melting point/freezing point

Not available.

Initial boiling point and boiling range

224.6 °F (107 °C) at 2.666 hPa

Flash point

104.0 - 129.9 °F (40.0 - 54.4 °C) (method not specified)

Evaporation rate

Not available.

Flammability (solid, gas)

Not applicable.

Upper/lower flammability or explosive limits

Flammability limit - lower (%)

Not available.

Flammability limit - upper (%)

Not available.

Explosive limit - lower (%)

Not available.

Explosive limit - upper (%)	Not available.
Vapor pressure	0.003 kPa (77 °F (25 °C))
Vapor density	Not available.
Relative density	Not available.
Solubility(ies)	
Solubility (water)	Slightly miscible. Insoluble.
Solubility (other)	Chloroform: Slightly soluble. Methanol: Slightly soluble.
Partition coefficient (n-octanol/water)	3.59 = log Pow at 21 °C
Auto-ignition temperature	> 1058 °F (> 570 °C)
Decomposition temperature	Not available.
Viscosity	Not available.
Other information	
Chemical family	Ketone.
Molecular formula	C12H16O
Molecular weight	176.25
Specific gravity	0.96 (water=1)

10. Stability and reactivity

Reactivity	The product is stable and non-reactive under normal conditions of use, storage and transport.
Chemical stability	Material is stable under normal conditions.
Possibility of hazardous reactions	No dangerous reaction known under conditions of normal use.
Conditions to avoid	Contact with incompatible materials. Ignition sources.
Incompatible materials	Strong oxidizing agents. Strong bases. Strong oxidizing agents.
Hazardous decomposition products	Irritating and/or toxic fumes or gases. Emits toxic fumes under fire conditions.

11. Toxicological information

Information on likely routes of exposure

Inhalation	Knowledge about health hazard is incomplete.
Skin contact	May cause an allergic skin reaction.
Eye contact	Causes eye irritation.
Ingestion	Knowledge about health hazard is incomplete.

Symptoms related to the physical, chemical and toxicological characteristics Not available.

Information on toxicological effects

Acute toxicity

Product	Species	Test Results
Ibuprofen Related Compound C (CAS 38861-78-8)		
<u>Acute</u>		
Oral		
LD50	Mouse	> 1600 mg/kg
	Rabbit	> 2000 mg/kg
	Rat	5000 mg/kg
Skin corrosion/irritation	Based on available data, the classification criteria are not met.	
Serious eye damage/eye irritation	Causes eye irritation.	

Local effects

Eye irritation test
Result: Slightly irritant.
Species: Rabbit
Skin irritation test
Result: Slightly irritant.
Species: Rabbit

Respiratory or skin sensitization

Respiratory sensitization Knowledge about sensitization hazard is incomplete.

Skin sensitization Knowledge about health hazard is incomplete.

Buehler Test
Result: Non-sensitizing.
Species: Guinea pig
Guinea Pig Maximization Test
Result: Sensitizing.

Germ cell mutagenicity Knowledge about mutagenicity is incomplete.

Mutagenicity

S. typhimurium Ames assay
Result: Negative.

Carcinogenicity Knowledge about carcinogenicity is incomplete.

IARC Monographs. Overall Evaluation of Carcinogenicity

Not listed.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1053)

Not listed.

US. National Toxicology Program (NTP) Report on Carcinogens

Not listed.

Reproductive toxicity Knowledge about health hazard is incomplete.

Specific target organ toxicity - single exposure Knowledge about health hazard is incomplete.

Specific target organ toxicity - repeated exposure Knowledge about health hazard is incomplete.

Aspiration hazard Knowledge about health hazard is incomplete.

Further information Pharmaceutical related compound of unknown potency. It is not known if occupational exposure may cause physiological effects.

12. Ecological information

Ecotoxicity

Product	Species		Test Results
Ibuprofen Related Compound C (CAS 38861-78-8)			
Acute			
Other	IC50	Pseudokirchnerella subcapitata	4 mg/l, 96 hours
Aquatic			
Acute			
Crustacea	EC50	Daphnia magna	7.7 mg/l, 48 hours
Fish	LC50	Bluegill (Lepomis macrochirus)	12.4 mg/l, 96 hours

Persistence and degradability No data is available on the degradability of this substance.

Bioaccumulative potential

Octanol/water partition coefficient log Kow
3.59, at 21 °C

Mobility in soil No data available.

Other adverse effects No other adverse environmental effects (e.g. ozone depletion, photochemical ozone creation potential, endocrine disruption, global warming potential) are expected from this component.

13. Disposal considerations

Disposal instructions Dispose in accordance with all applicable regulations. Under RCRA, it is the responsibility of the user of the product to determine, at the time of disposal, whether the product meets RCRA criteria for hazardous waste.

Local disposal regulations

Dispose in accordance with all applicable regulations.

Hazardous waste code

D001: Waste Flammable material with a flash point <140 F

The waste code should be assigned in discussion between the user, the producer and the waste disposal company.

Waste from residues / unused products

Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe manner (see: Disposal instructions).

Contaminated packaging

Since emptied containers may retain product residue, follow label warnings even after container is emptied.

14. Transport information**DOT**

UN number	UN1224
UN proper shipping name	Ketones, liquid, n.o.s. (Ethanone, 1-[4-(2-methylpropyl)phenyl]-)
Transport hazard class(es)	
Class	3
Subsidiary risk	-
Packing group	III

IATA

UN number	UN1224
UN proper shipping name	Ketones, liquid, n.o.s. (Ethanone, 1-[4-(2-methylpropyl)phenyl]-)
Transport hazard class(es)	
Class	3
Subsidiary risk	-
Packing group	III

Other information

Passenger and cargo aircraft Allowed with restrictions.

Cargo aircraft only Allowed with restrictions.

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

Not established.

DOT**IATA****General information**

It is the shipper's responsibility to determine the correct transport classification at the time of shipment.

15. Regulatory information**US federal regulations**

This product is a "Hazardous Chemical" as defined by the OSHA Hazard Communication Standard, 29 CFR 1910.1200.

Toxic Substances Control Act (TSCA)

TSCA Section 12(b) Export Notification (40 CFR 707, Subpt. D)

Not regulated.

CERCLA Hazardous Substance List (40 CFR 302.4)

Not listed.

SARA 304 Emergency release notification

Not regulated.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1053)

Not listed.

Superfund Amendments and Reauthorization Act of 1986 (SARA)**SARA 302 Extremely hazardous substance**

Not listed.

SARA 311/312 Hazardous chemical

Classified hazard categories	Flammable (gases, aerosols, liquids, or solids) Serious eye damage or eye irritation Respiratory or skin sensitization
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SARA 313 (TRI reporting)

Not regulated.

Other federal regulations**Clean Air Act (CAA) Section 112 Hazardous Air Pollutants (HAPs) List**

Not regulated.

Clean Air Act (CAA) Section 112(r) Accidental Release Prevention (40 CFR 68.130)

Not regulated.

Safe Drinking Water Act (SDWA)

Not regulated.

US state regulations**California Proposition 65**

California Safe Drinking Water and Toxic Enforcement Act of 1986 (Proposition 65): This material is not known to contain any chemicals currently listed as carcinogens or reproductive toxins. For more information go to www.P65Warnings.ca.gov.

International Inventories

Country(s) or region	Inventory name	On inventory (yes/no)*
Australia	Australian Inventory of Chemical Substances (AICS)	No
Canada	Domestic Substances List (DSL)	No
Canada	Non-Domestic Substances List (NDSL)	Yes
China	Inventory of Existing Chemical Substances in China (IECSC)	No
Europe	European Inventory of Existing Commercial Chemical Substances (EINECS)	Yes
Europe	European List of Notified Chemical Substances (ELINCS)	No
Japan	Inventory of Existing and New Chemical Substances (ENCS)	Yes
Korea	Existing Chemicals List (ECL)	No
New Zealand	New Zealand Inventory	No
Philippines	Philippine Inventory of Chemicals and Chemical Substances (PICCS)	No
Taiwan	Taiwan Chemical Substance Inventory (TCSI)	Yes
United States & Puerto Rico	Toxic Substances Control Act (TSCA) Inventory	Yes

*A "Yes" indicates that all components of this product comply with the inventory requirements administered by the governing country(s)

A "No" indicates that one or more components of the product are not listed or exempt from listing on the inventory administered by the governing country(s).

16. Other information, including date of preparation or last revision

Issue date 11-12-2009

Revision date 09-21-2021

Version # 07

Disclaimer

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