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**KAMPOYAKI NATURAL
PRODUCTS BIO-CHEMISTRY**

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3-BUTYLIDENEPHTHALIDE

Datasheet

Kampoyaki Novo-Drug Screening Libraries 4th Edition (Revised in July, 2016)

PRODUCT INFORMATION

Name: 3-Butylidenephthalide

Catalog No.: KRN99588

Cas No.: 551-08-6

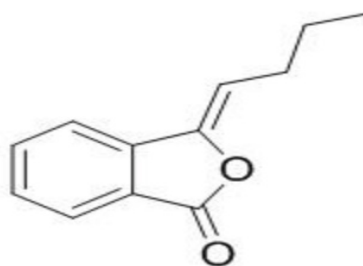
Purity: >=98%

M.F: C₁₂H₁₂O₂

M.W: 188.22

Physical Description: Oil

Synonyms: 3-Butylidene-1(3H)-Isobenzofuranone; Butylidenephthalide.



POTENTIAL USES

1. Reference standards; **2.** Pharmacological research; **3.** Food and cosmetic research;
4. Synthetic precursor compounds; **5.** Active Pharmaceutical Intermediates (API) & Fine Chemicals; **6.** Ingredient in supplements, beverages; **7.** Agricultural research; **8.** Botanical Bio- Allelopathy, **9.** Natural Botanical Molecules as Botanical Bio-Herbicides **10.** As Botanical Bio- Anti-Blight Fungicides

SOURCE

The roots of Ligusticum chuanxiong hort.

BIOLOGICAL ACTIVITY OR INHIBITORS

Butylidenephthalide (BDPH) is one of the most potent vasorelaxants isolated from *Ligusticum chuanxiong* Hort, BDPH-mediated vasorelaxation comprises both endothelium-dependent (NO) and independent components, suggests that BDPH acting through an inhibitory mechanism downstream to I-type voltage-operated and prostanoid TP receptor-operated Ca²⁺ channels operating late in the contractile pathway.[1] 3-(Z)-butylidenephthalide shows antihyperglycemic activity, its antihyperglycemic effect is due to inhibition of α -glucosidase at the intestinal level, it inhibits the activity of yeast- α -glucosidase (IC₅₀ 2.35 mM) in a noncompetitive fashion with a K_i of 4.86 mM.[2]

(E)- and (Z)-Butylidenephthalide have insecticidal and acaricidal activities, they exhibits 50% lethal concentration (LC₅₀) values of 2.07 and 0.94 micromol/ml of diet concentration against larvae of *D. melanogaster*, respectively. [3]

Butylidenephthalide inhibits, in a dose-dependent manner, the aggregation and release reaction of washed rabbit platelets induced by collagen and arachidonic acid, the antiplatelet effect of butylidenephthalide is mainly due to an inhibitory effect on cyclo-oxygenase and may be due partly to interference with calcium mobilization.[4]

Butylidenephthalide significantly enhances tension in isolated guinea-pig trachea. In this study, it may be similar to 4-AP, a blocker of Kv1 family of K⁺ channels, to enhance the baseline tension of guinea-pig trachea.[5]

Butylidenephthalide, an antispasmodic compound, it has a selective anti-anginal effect without changing blood pressure, it inhibits calcium release from calcium stores more selectively than calcium influx from extracellular space via voltage-dependent calcium channels, the inhibition by it of calcium release from KCl-sensitive calcium stores may be similar to its inhibition of calcium release from phenylephrine-sensitive calcium stores. [6]

SOLVENT

Pyridine, Methanol, Ethanol, Hot water, etc.

HPLC METHOD (7)

Mobile phase: Methanol - H₂O, gradient elution ;

Flow rate: 1.0 ml/min;

Column temperature: Room Temperature;

The wave length of determination: 270 nm.

STORAGE

2-8°C, Protected from air and light, refrigerate or freeze.

REFERENCES

- [1] Chan S K, Choi O K, Jones R L, et al. *Eur. J. Pharmacol.*, 2006, 537(1-3):111-7.
- [2] Brindis F, Rodríguez R, Bye R, et al. *J. Nat. Prod.*, 2011, 74(3):314-20.
- [3] Tsukamoto T, Nakatani S Y, Sakai N, et al. *Biol. Pharmaceut. Bull.*, 2006, 29(3):592-4.
- [4] Teng C M, Chen W Y, Wun-Chang K O, et al. *B.B.A.-Gen.Subjects*, 1987, 924(3):375-82.
- [5] Hsin-Te Hsu, Yang Y L, Chen W C, et al. *Biomed. Res. Int.*, 2014, 2014(3):1153-66.
- [6] Ko W C, Charng C Y, Sheu J R, et al. *J. Pharm. Pharmacol.*, 1998, 50(12):1365-9.
- [7] Li H X, Ding M Y, Yu J Y. *J. Chromatogr. Sci.*, 2002, 40(3):156-61.



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CERTIFICATE OF ANALYSIS

Name: 3-Butylidenephthalide

Catalog No.: KRN99588

Cas No.: 551-08-6

Purity: >= 98%

M.F: C₁₂H₁₂O₂

Physical Description: Oil

Solvent: Pyridine, Methanol, Ethanol, etc.

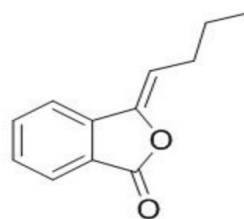
Weight 20mg

Lot No. KRS201901

Storage Protected from air and light, refrigerate or freeze (2-8 °C)

Intended Use For laboratory use only

Shelf Life 2 years



CHARACTERIZATION DATA SUMMARY

Analytical Test

Identification by ¹H-NMR ,
Purity tested

Results

Consistent with the above structure
>= 98%



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GHS SAFETY DATA SHEET

Version 4.2

Revision Date 01/01/2018

Print Date 01/08/2019

1. PRODUCT AND COMPANY IDENTIFICATION

GHS Product Name: 3-Butylidenephthalide

Product code: KRN99588

Company: KAMPOYAKI HERS PTE LTD

Address: 16 New Industrial Road, #05-05 Hudson Techno Centre Singapore 536204

Tel: +65-63833202

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2. HAZARDS IDENTIFICATION

2.1 GHS classification

Physical Hazards: Not classified

Health Hazards: Not classified

Environmental Hazards: Not classified

2.2 GHS label elements, including precautionary statements

Pictograms or hazard symbols: None

Signal word: No signal word

Hazard statements: None

Precautionary statements: None

3. COMPOSITION/INFORMATION ON INGREDIENTS

Chemical Name: 3-Butylidenephthalide

CAS#: 551-08-6

Purity: $\geq 98\%$

Formula: $C_{12}H_{12}O_2$

Molecular Weight: 188.22

Hazard Symbols: ---

Risk Phrases: ---

4. FIRST AID MEASURES

4.1 Description of first aid measures

Eyes: Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Consult a doctor.

Skin: Flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Consult a doctor.

Ingestion: Do NOT induce vomiting. If conscious and alert, rinse mouth and drink 2-4 cupfuls of milk or water. Consult a doctor.

Inhalation: Remove from exposure and move to fresh air immediately. Consult a doctor.

4.2 Indication of immediate medical attention and special treatment needed

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

5. FIRE FIGHTING MEASURES

5.1 Suitable extinguishing

Media: Dry chemical, foam, water spray, carbon dioxide.

Precautions for firefighters: Fire-extinguishing work is done from the windward and the suitable fire-extinguishing method according to the surrounding situation is used. Uninvolved persons should evacuate to a safe place. In case of fire in the surroundings: Remove movable containers if safe to do so.

5.2 Special protective

Equipment for firefighters: When extinguishing fire, be sure to wear personal protective equipment.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing vapors, mist or gas.

6.2 Environmental precautions

Do not let product enter drains.

6.3 General Information

Use proper personal protective equipment as indicated in Section 8.

6.4 Spills/Leaks

Clean up spills immediately, observing precautions in the Protective Equipment section. Sweep up, then place into a suitable container for disposal. Decontaminate spill site with 10% caustic solution and ventilate area until after disposal is complete

7. HANDLING AND STORAGE

7.1 Precautions for safe handling:

Wash thoroughly after handling. Remove contaminated clothing and wash before reuse. Avoid contact with eyes, skin, and clothing. Avoid ingestion and inhalation. Keep away from sources of ignition. Avoid prolonged or repeated exposure.

7.2 Storage

Store in a well closed container. Protected from air and light, refrigerate or freeze.(2-8°C)

7.3 Specific end uses

Use in a laboratory fume hood where possible. Refer to employer is COSHH risk assessment.

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

8.1 Engineering controls

Use adequate general or local exhaust ventilation to keep airborne concentrations below the permissible exposure limits. Use process enclosure, local exhaust ventilation, or other engineering controls to control airborne levels.

Control parameters: Not set up

8.2 Personal protective equipment

Respiratory protection: Dust respirator. Follow local and national regulations.

Hand protection: Protective gloves.

Eye protection: Wear safety glasses and chemical goggles if splashing is possible.

Skin and body protection: Wear appropriate protective gloves and clothing to prevent skin exposure.

9. PHYSICAL AND CHEMICAL PROPERTIES

- a) Appearance Yellow powder
- b) Odour no data available
- c) Odour Threshold no data available
- d) pH no data available
- e) Melting point/freezing point no data available
- f) Initial boiling point and boiling range no data available
- g) Flash point no data available
- h) Evaporation rate no data available
- i) Flammability (solid, gas) no data available
- j) Flammability or explosive limits no data available
- k) Vapour pressure no data available
- l) Vapour density
- m) Relative density no data available
- n) Water solubility no data available
- o) Partition coefficient: no data available
- p) Autoignition temperature no data available
- q) Decomposition temperature no data available
- r) Viscosity no data available
- s) Explosive properties no data available
- t) Oxidizing properties no data available

10 - STABILITY AND REACTIVITY

10.1 Reactivity

Stable under recommended transport or storage conditions.

10.2 Chemical Stability

Stable under normal temperatures and pressures.

10.3 Conditions to Avoid

Incompatible materials, strong oxidants, heat.

10.4 Incompatibilities with Other Materials

Strong oxidising/reducing agents, strong acids/alkalis.

10.5 Hazardous Decomposition Products

Nitrogen oxides, carbon monoxide, irritating and toxic fumes and gases, carbon dioxide, nitrogen.

10.6 Hazardous Polymerization

Has not been reported.

11. TOXICOLOGICAL INFORMATION

Acute Toxicity:	No data available
Skin corrosion/irritation:	No data available
Serious eye damage/irritation:	No data available
Germ cell mutagenicity:	No data available
Carcinogenicity:	---
IARC:	No data available
NTP:	No data available
Reproductive toxicity:	No data available

12. ECOLOGICAL INFORMATION

Toxicity:	No data available
Persistence and degradability:	No data available
Bioaccumulative potential:	No data available
Mobility in soil:	No data available
Results of PBT and vPvB assessment:	No data available
Other adverse effects:	May be harmful to the aquatic environment.

13. DISPOSAL CONSIDERATIONS

Dispose of in a manner consistent with federal, state, and local regulations.

14. TRANSPORT INFORMATION

14.1 Hazards Class:

Does not meet the criteria for classification as hazardous for transport

14.2 UN proper shipping name

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA: Not dangerous goods

14.3 Transport hazard class(es)

Does not meet the criteria for classification as hazardous for transport.

15. REGULATORY INFORMATION

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

No data available

15.2 Chemical Safety Assessment

No data available

16. ADDITIONAL INFORMATION

This GHS SDS above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no way shall the company be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if the company has been advised of the possibility of such damages.

End of GHS safety data sheet



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