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NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME

FULL PUBLIC REPORT

2-(phenylmethoxy) naphthalene

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Director
Chemicals Notification and Assessment

FULL PUBLIC REPORT

2-(phenylmethoxy) naphthalene

1. APPLICANT

Amcor Trading Pty Ltd of Floor 2, 570 St Kilda Road, Melbourne, Victoria, has applied for a standard notification for assessment of 2-(phenylmethoxy) naphthalene (BNE).

2. IDENTITY OF THE CHEMICAL

Chemical name: 2-(phenylmethoxy) naphthalene

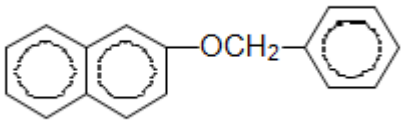
Chemical Abstracts Service (CAS) Registry No.: 613-62-7

Other name: Benzyl 2-naphthyl ether

Trade name: BNE

Molecular formula: $C_{17}H_{14}O$

Structural formula:



Molecular weight: 234

Method of detection and determination:

UV, NMR & FT-IR

Spectral data:
UV/Vis spectrum: major peaks at230 nm (2.5 μg/ml)
262, 272, 312, 328 nm (24.8 μg/ml)

IR/Spectrum: major peaks at 3463.8, 3449.2, 3060.0/, 3028.2, 2933.2, 1627.4, 1598.7, 1512.0, 1390.5, 1257.9, 1217.6, 1179.9, 1023.1, 1019.1, 840.2, 744.9, 692.2, 479.9 cm^{-1}.

3. PHYSICAL AND CHEMICAL PROPERTIES

Appearance at 20ºC and 101.3 kPa:	Fine white powder
Odour:	Not provided
Melting Point:	101.1-102.6°C
Boiling Point:	148~150°C/1.3-0.7 Pa
Relative Density:	1.27
Vapour Pressure:	5.6×10^{-5} Pa at 20°C
Water Solubility:	0.078 ± 0.013 mg/L (20°C)
Partition Co-efficient (n-octanol/water):log P_{ow}	4.46 (20°C)
Fat Solubility:	5647 ± 379 mg/100 g fat simulant 307 (37°C).
Hydrolysis as a function of pH:	Low water solubility is likely to inhibit hydrolysis. There are also no groups considered likely to hydrolyse under environmental conditions.
Adsorption/Desorption:	Not provided.
Dissociation Constant:	The low water solubility and lack of ionisable groups indicate the notified chemical is unlikely to dissociate.
Flash Point:	Not provided
Flammability Limits:	Not flammable
Combustion Products:	Complete combustion products are carbon dioxide and water
Decomposition Temperature:	Not provided
Decomposition Products:	Not provided
Autoignition Temperature:	Not provided
Explosive Properties:	Not explosive when exposed to flame

Reactivity/Stability: Not an oxidiser

Particle size distribution: Not provided

4. PURITY OF THE CHEMICAL

Degree of purity: > 99%

Toxic impurities: None

Non-toxic impurities:(> 1% by weight)

Chemical name: Benzyl 2-benzyloxy-naphthalene
Weight percentage: < 1%

Additives/Adjuvants: None

5. INDUSTRIAL USE

The notified chemical, in the form of a fine white powder, is a colour forming agent for use in specialty papers, such as chemithermal papers. It is expected that between 10 and 100 tonnes per annum will be imported in the first five years.

6. OCCUPATIONAL EXPOSURE

The notified chemical will be imported into Australia in fibre kegs or paper bags and will be incorporated into a paper coating at a single site. The chemical is firstly dispersed into water with other powdered and granular water insoluble raw materials in a robust, stainless steel mixing vessel. The chemical is charged manually from bags into the mixing vessel by 3 process workers. The chemical is at 20% in this first mix with worker exposure at a maximum of 1/2 hour per day on up to about 60 days per year. The mixture is then recirculated automatically through a closed grinding mill back to the mixing vessel. The milled mixture is then transferred via pipeline and air diaphragm pump to another stainless steel slow speed mixing vessel containing a paper coating preparation. The chemical is now at level of 5%.

The paper coating is taken manually from the mixing vessel via 20 litre buckets to the paper coating machine by any of the 4 printers, 2 apprentice printers or 4 printers assistants at a rate of one bucket every 15 minutes and discharged into the coating machine's coating circulation tank. Maximum exposure by any one person at this stage is 2 hours/day.

The wet coating is then automatically applied to the paper by the coating machine. The paper is dried (at 60ºC max through hot air ovens which exhaust to outside the factory) and then automatically wound into reels. The chemical is now at a maximum of 1.5% on the coated paper and is bound within the coating on the paper surface with polyvinyl alcohol binders.

The reels of coated paper are next slit into smaller reels and packaged for distribution and use in thermal printing machines. This is done either in-house or by outside converting companies. In-house, 2 converter operators and 2 packers (at any one time) handle small rolls for a maximum of 4 hours/day. Up to 20 external companies who have converting operations could be converting coated paper containing this chemical. Exposure by workers at these companies is not expected to be greater than for the in-house converting operation.

Exposure of 3 laboratory staff is limited to those doing quality assurance on the milled mixture and final paper coating as well as those handling samples of the coated paper. Maximum exposure would be 4 hours/day for 1 person.

7. PUBLIC EXPOSURE

The notified chemical will be used as a colour forming agent in speciality papers, such as chemithermal papers (eg facsimile paper) and will constitute up to 1.5% of finished products.

The notified chemical will be distributed to manufacturers of thermal paper and no public exposure is expected to occur during its distribution.

No significant public exposure to the notified chemical during the manufacture of thermal paper is expected to occur. However, public contact with the notified chemical resulting from use of treated paper is expected to be extensive.

Disposal of waste chemical will involve chemical treatment and/or destruction via a chemical incinerator, and no significant public exposure is expected to occur.

8. ENVIRONMENTAL EXPOSURE

. Release

The quantity of notified chemical contained in waste cleaning water from the paper coating site is estimated to be 0.5 kg/day. This waste is suspended in water discharge (after washing out mixing vessels and coating units) to the sewer system via a Victorian Board of Works recommended triple interceptor separation pit. The estimated concentration of release to the sewer is 250 ppm.

The notified chemical is a maximum of 1.5% of the finished products which when used are either filed for future reference or treated as waste paper. Releases to the environment may occur through processing of waste paper. This possibility is explored further below.

. Fate

When the notified chemical is discharged from the paper coating plant to sewer it is likely to be adsorbed to suspended solids based on its low water solubility and octanol-water

partition coefficient. The chemical is unlikely to biodegrade at sewage treatment plants (see below) and is likely to become associated with the sludge.

Disposal of the notified chemical to landfill is unlikely to result in contamination of surface and ground waters. Its low water solubility and high Log P_{ow} indicates it is unlikely to leach.

Combustion of the notified chemical in the presence of excess air will result in products of oxides of carbon and water.

Unless incinerated, the notified chemical is likely to arrive in a dispersed manner in landfill bound to waste paper which would limit accumulation. As such, it will be immobile, and no leaching from landfill would be expected despite the chemical's expected persistence (see below).

- Paper recycling

Paper recycling is a growing industry in Australia. Wastepaper is repulped using a variety of alkalis, dispersing agents, wetting agents, water emulsifiable organic solvents and bleaching agents. These chemicals enhance fibre separation, ink detachment from the fibres, pulp brightness and whiteness of the paper. After pulping, the contaminants and the ink are separated from the fibres by pumping the stock through various heat washing, screening, cleaning, flotation and dispersion stages. The chemical is likely to survive the above conditions, either remaining bound to the pulp or becoming associated with the sludge. In the latter case, the chemical will either arrive in landfill where it can be expected to remain intact and is likely to accumulate, or be destroyed through incineration.

- Biodegradation

The biodegradability of BNE was determined by the Modified Sturm Test (OECD TG 301B) (1) at two concentrations, 12.3 mg/L and 23 mg/L. The notified chemical, along with inoculated medium (activated sludge), were incubated for 28 days. At the end of the study, CO_2 production was only recorded from the higher test concentration, at a level of 1% of the theoretical CO_2 for BNE. Therefore, BNE is not readily biodegradable.

BNE was further investigated for its biodegradability in the Modified MITI-Test (II) - OECD TG 302C (2). The notified chemical (30 mg/L) was inoculated with activated sludge and incubated in flasks for 28 days in darkness at 25°C. The oxygen demand of the flasks containing the test article remained equal to or below the inoculum blanks throughout the exposure period. Therefore, BNE was found to be non-degradable under the test conditions which examined inherent biodegradability.

- Bioaccumulation

The bioaccumulation potential of BNE was investigated in Bluegill sunfish by means of a dynamic flow-through system (OECD TG 305E) (3). The fish were continuously exposed to ^{14}C-BNE at an average low dose concentration of 7.6 µg/L and an average high dose concentration of 76 µg/L for 7 days. Thereafter the fish were transferred to flowing

untreated water and the depuration of radioactivity followed for 14 days. BNE reached plateau levels in the fish and fish parts within 58-120 hours continuous exposure and rapidly depurated with half-lives of 11-16 hours, resulting in bioconcentration factors for BNE of 38-84 for edibles, 203-431 for non-edibles and 180-270 for the whole fish. The results indicate that BNE is unlikely to bioaccumulate significantly in fish.

9. EVALUATION OF TOXICOLOGICAL DATA

9.1 Acute Toxicity

Table 1 Summary of the acute toxicity of BNE

Test	Species	Outcome	Reference
Acute oral toxicity	Rat	LD_{50} > 2000 mg/kg	(4)
Acute dermal toxicity	Rat	LD_{50} > 2000 mg/kg	(5)
Skin Irritation	Rabbit	slight irritant	(6)
Eye irritation	Rabbit	slight irritant	(8)
Skin sensitisation	Guinea-pig	Non-sensitiser	(9)

All tests were conducted in accordance with OECD guidelines (10).

9.1.1 Oral Toxicity (4)

SD rats (5/sex) were administered a single gavage dose of BNE at 2000 mg/kg in maize oil (20% w/v) and were then observed for 14 days. No deaths, clinical signs of toxicity or treatment-related macroscopic lesions were observed. The oral LD_{50} of BNE was > 2000 mg/kg. The results of the study indicate that BNE has low oral toxicity.

9.1.2 Dermal Toxicity (5)

SD rats (5/sex) were dermally (intact skin) treated with BNE at 2000 mg/kg in maize oil (20% w/v). The treated site was maintained under occlusive dressing (plastic film) for 24 hours. The observation period was 14 days. No deaths or signs of toxicity were observed. The dermal LD_{50} of BNE in rats was > 2000 mg/kg. The results of the study indicate that BNE has low dermal toxicity.

9.1.3 Skin Irritation (6)

Three NZW rabbits were dermally (intact skin) exposed to 0.5 g of BNE in 0.5 g of tap water in a small plastic cup for 4 hours. One hour after exposure, very slight erythema with or without very slight oedema was observed in all three rabbits. Average Draize (7) scores for erythema and oedema were 1.0 and 0.7, respectively. After 24 hours there were no signs of skin irritation reported. The results of the study indicate that BNE is a slight skin irritant in rabbits.

9.1.4 Eye Irritation (8)

Three NZW rabbits were treated with 0.1 mL (0.065 g) of BNE by instillation into the conjunctival sac of one eye. One hour after exposure, only slight redness and swelling of the conjunctivae and slight ocular discharge were reported. Average Draize scores for conjunctival oedema and chemosis, and ocular discharge were 0.33. After 24 hours there were no signs of ocular irritation reported. The results of this study indicate that BNE is a slight eye irritant in rabbits.

9.1.5 Skin Sensitisation (9)

The skin sensitisation potential of BNE was studied in guinea-pigs using the maximisation test of Magnusson and Kligman (11).

Bor:DHPW guinea-pigs were induced by intradermal injections of Freund's Complete Adjuvant (FCA), a 10% dilution of the test substance in maize oil, and a 10% dilution of the test substance in a mixture (1:1) of FCA and maize oil, followed one week later by topical application of a 50% dilution of the test substance in demineralised water for 24 hours. Fourteen days following the last induction, animals were challenged with a 50% dilution of the test substance in demineralised water for 48 hours. A group of control animals were similarly treated but the test substance was omitted.

The challenge treatment induced very slight erythema in 5/20 test animals and in 1/10 controls. On the basis of similarities between the type of skin reactions occurring in test and control groups, the results of a preliminary skin irritation study in which a 50% test dilution produced irritation in 1/3 animals tested, and the nature and degree of the skin reactions normally observed after challenging with standard allergens, the skin reactions in this study were considered to be consistent with signs of skin irritation rather than sensitisation. The results of this study indicate that BNE is not a skin sensitiser in guinea-pigs.

9.2 Repeated Dose Toxicity (12)

SD rats (5/sex/group) were administered BNE at 0, 3, 30 or 300 mg/kg for 28 days by gavage. Dose levels were selected on the basis of a 5 day dose range finding study in which increased liver weights occurred in males at 1000 mg/kg/d and in females from 100 mg/kg/d. In the 28-day study, there were no deaths or treatment-related clinical signs reported. Body weight gain, food and water consumption, and haematological parameters were not affected by treatment. Changes in clinical chemistry parameters included increased bilirubin in males and females given 300 mg/kg/d, and in males decreased cholesterol at 300 mg/kg/d and increased gamma glutamyl transferase activity from 30 mg/kg/d. Liver weights in females were increased at 300 mg/kg/d, and at 30 and 300 mg/kg/d discolouration of the urine occurred in both sexes. There were no other effects attributed to treatment. The results of this study indicate that while BNE produces effects suggestive of hepatotoxicity, it is not classed as harmful or toxic.

9.3 Genotoxicity

9.3.1 *Salmonella typhimurium* Reverse Mutation Assay (13)

Salmonella typhimurium strains TA98, TA100, TA1535, TA1537 and TA1538 were cultured with BNE at 25 - 2000 ug/plate with or without metabolic activation provided by rat liver S9. All dose levels were plated in triplicate. Vehicle (DMSO) and positive controls were run concurrently. In the positive controls, 2-aminoanthracene was used in the presence of S9 in all the strains and in the absence of S9, 2-nitrofluorene was used in strains TA98 and TA1538, sodium azide in strains TA100 and TA1535, and 2-aminoacridine in strain TA1537. At the highest test concentration, precipitation occurred and cytotoxicity was reported in all strains in the presence or absence of metabolic activation. No reproducible increases in mutant frequency were reported in any of the treatment or vehicle control groups. The positive controls produced marked increases in mutant frequency in all the test strains. Under the conditions of the assay, BNE was not mutagenic in the *Salmonella typhimurium* reverse mutation assay.

9.3.2 *In vitro* mammalian cytogenetic test in Chinese hamster cells. (14)

Chinese hamster ovary cells were treated with BNE (in DMSO) at 0, 1, 3, 10, 30, or 100 ug/mL for 21 hours in the absence of metabolic activation, and at 0, 1, 10, 12.5, 15, 17.5 or 20 µg/mL for 3 hours in the presence of metabolic activation provided by rat liver S9. The two highest concentrations used in the presence of metabolic activation (17.5 and 20 ug/mL) were only used to determine the mitotic index. Mitomycin C (0.05 ug/mL) and cyclophosphamide (100 ug/mL) were used as positive controls in the absence and presence of metabolic activation, respectively. Cells were harvested after 21 hours in the absence of metabolic activation and after 12 and 21 hours in the presence of metabolic activation. Two hours prior to harvesting, the cells were arrested in metaphase with the addition of colcemid at 0.1 ug/mL of medium, and slides were prepared for metaphase analyses. Treatment of cells in the absence or presence of metabolic activation did not result in an increase in chromosomal aberrations. Cytotoxicity was reported from 10 ug/mL and 12.5 ug/mL in the absence and presence of metabolic activation, respectively. The positive controls induced the expected increase in the incidence of structural chromosome aberrations. BNE did not induce structural chromosomal aberrations in CHO cells in this study.

9.3.3 Micronucleus Assay in the Bone Marrow Cells of the Mouse (15)

NMRI mice (5-10/sex/group) were intraperitoneally administered 0, 200, 670 or 2000 mg/kg of BNE, suspended in corn oil. A positive control group (5/sex) was treated with 30 mg/kg of cyclophosphamide. Bone marrow was collected from treatment and control mice after approximately 24 hours, and from mice given 2000 mg/kg and the vehicle control after 48 hours. Bone marrow smears were made from each animal and 1000 polychromatic erythrocytes were scored for micronuclei. No clinical signs of toxicity were reported during the study, however in a preliminary toxicity study, signs of toxicity occurring at 2000 mg/kg/d included reduction of spontaneous activity, eyelid closure and apathy for up to 6 hours following treatment. No cytotoxicity was reported in any treatment or control assays. No significant increase in the number of micronucleated polychromatic erythrocytes was reported in treatment assays. The positive control induced micronuclei

as expected. BNE did not cause chromosomal damage in bone marrow cells of the mouse *in vivo* in this study.

9.4 Overall Assessment of Toxicological Data

Based on the toxicity studies provided by the notifier, BNE was of low acute oral and dermal toxicity in rats, it was a slight irritant to the skin and eyes of rabbits and was not demonstrated to be a skin sensitiser in guinea-pigs. Repeated administration of BNE to rats at up to 300 mg/kg/day orally for 28 days produced effects suggestive of hepatotoxicity from 30 mg/kg/d . This was not supported by any microscopic changes in normal liver structure. BNE was not mutagenic in *S.typhimurium* in an *in vitro* bacterial reverse mutation assay, did not cause chromosomal damage in Chinese hamster ovary cells *in vitro*, and did not cause chromosomal damage in mouse bone marrow cells *in vivo*.

BNE would not be classified as hazardous according to Worksafe Australia's *Approved Criteria for Classifying Hazardous Substances* (16) in relation to Acute lethal effects (oral, dermal); Irritant effects (skin, eye), Sensitising effects (skin), Severe effects after repeated or prolonged exposure or Mutagenic effects.

10. ASSESSMENT OF ENVIRONMENTAL EFFECTS

The following ecotoxicity studies have been provided by the notifier.

Table 2 Summary of Environmental Effects of BNE

Test (reference)	Species	Result
Acute toxicity (17)	Freshwater fish *Brachydanio rerio*	96h LC_{50} > 100 mg/L NOEC > 100 mg/L
Acute toxicity (18)	*Daphnia magna*	24h EC_{50} > 100 mg/L NOEC > 100 mg/L
Growth inhibition (19)	Algae *Scendesmus subspicatus*	96h EC_{50} > 90 µg/L NOEC > 70 µg/L

The above studies were conducted according to OECD test guidelines. The results are based on nominal concentrations due to the low solubility of the chemical is water. DMSO (dimethyl sulphoxide) was used as a solvent in the fish and daphnia studies, but the solutions were turbid and undissolved particles were observed on the bottom of the test vessels. For the algae study, a supersaturated solution of BNE was filtered and the filtrate used as the test solution.

The studies indicate that toxicity of BNE is above its water solubility (78 ppb) and therefore is unlikely to have adverse effects on aquatic organisms. The notifier claims that the EC_{50} for parental immobility and reproduction for daphnia exceed the maximum solubility of BNE in water. However, no study report was provided to confirm the result.

11. ASSESSMENT OF ENVIRONMENTAL HAZARD

When the notified chemical is discharged from the paper coating plant to sewer it is likely to be adsorbed to suspended solids and become associated with the sludge at sewerage treatment works (STW). Assuming that no adsorption occurred (worst-case situation) the concentration of the chemical discharged from the STW would be 2 ppb, based on 0.5 kg chemical diluted by metropolitan sewer flow of 250 mL/day. Further dilution in receiving waters would occur to levels of < 1 ppb. Therefore, the notified chemical is unlikely to present a hazard to aquatic organisms based on the ecotoxicity results provided.

The low environmental exposure of the chemical as a result of normal use indicates that the overall environmental hazard should be negligible.

Environmental exposure to the notified substance could occur when paper containing the chemical is recycled or disposed of. In each case, the final destination is likely to be landfill where the chemical can be expected to persist but remain immobile, being either bound to paper or to the sludge from the recycling process.

Accidental spillage of the notified chemical should result in negligible hazard as it will be marketed in small packages for direct insertion into photocopier machines.

12. ASSESSMENT OF PUBLIC AND OCCUPATIONAL HEALTH AND SAFETY EFFECTS

BNE is expected to exhibit low oral and dermal toxicity and be slightly irritating to skin and eyes. It is not expected to be a sensitising agent, to exhibit significant toxicity following repeated or prolonged exposure and is not expected to be genotoxic.

Occupational exposure to BNE in dust form may occur during transfer of the chemical to the initial tank for mixing. Exposure is also possible when the resultant solution in open buckets is transferred to the paper coating machine, otherwise the chemical will exist in a closed system or in a paper coating. The level of exposure is expected to be low under normal conditions of use.

There is a risk of slight respiratory, skin and eye irritation.

Although significant public contact to BNE is expected to occur as a result of using treated products, exposure levels will be low since BNE is at a level of 1.5% in the final coating. Based on the toxicological data submitted such low exposures are not expected to pose a health risk to the public.

13. RECOMMENDATIONS

To minimise occupational exposure to 2-(phenylmethoxy) naphthalene (BNE) the following guidelines and precautions should be observed:

- if engineering controls and work practises are insufficient to reduce exposure to a safe level, then personal protective devices which conform to and are in accordance with Australian (or Australian/New Zealand) Standards (AS or AS/NZS) for respiratory protection (face mask) (AS/NZS 1715) (20) chemical type goggles (AS 1336, AS 1337) (21,22), rubber gloves (AS 2161) (23) overalls (AS 2919) (24) and protective shoes (AS/NZS 2210) (25) should be worn.

- good work practises should be implemented to avoid spillages.

- disposal of waste should be in accordance with Material Safety Data Sheet (MSDS) recommendations and Local and State government regulations.

- good personal hygiene practices, such as washing of hands prior to eating food, should be observed.

- a copy of the MSDS for BNE and products containing it should be easily accessible to workers

14. MATERIAL SAFETY DATA SHEET

The attached Material Safety Data Sheet (MSDS) for 2-(phenylmethoxy) naphthalene (BNE) was provided in Worksafe Australia format (26).

This MSDS was provided by Amcor Trading Pty Ltd as part of their notification statement. The accuracy of this information remains the responsibility of Amcor Trading Pty Ltd.

15. REQUIREMENTS FOR SECONDARY NOTIFICATION

Under the *Industrial Chemicals (Notification and Assessment) Act 1989*, secondary notification of 2-(phenylmethoxy) naphthalene (BNE) shall be required if any of the circumstances stipulated under subsection 64(2) of the Act arise. No other specific conditions are prescribed.

16. REFERENCES

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16. National Occupational Health and Safety Commission 1994, *List of Designated Hazardous Substances [NOHSC10005(1994)].* Australian Government Publishing Service, Canberra.

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