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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**

Robert Bryce and Company Ltd. of 64 Trenerry Crescent, Abbotsford, Victoria, 3067 has applied for a standard notification for assessment of 2-(phenylmethoxy) naphthalene, (2- BON).

2. IDENTITY OF THE CHEMICAL

Chemical name: 2-(phenylmethoxy) naphthalene

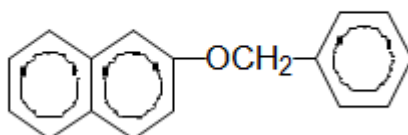
Chemical Abstracts Service (CAS) Registry No.: 613-62-7

Other name: ZO-1

Trade name: 2-BON

Molecular formula: C₁₇H₁₄O

Structural formula:



Molecular weight: 234

Method of detection and determination:

UV, NMR & FT-IR

Spectral data:

UV/Vis spectrum: major peak at 240 nm.

IR spectrum:

Wave Number (cm ⁻¹)	Attribution
3000	C-H aromatic hydrocarbon
2900	C-H benzyl group
1620 - 1480	C=C benzene ring
1200 - 1000	C-O ether
860 - 680	C-H aromatic ring

3. PHYSICAL AND CHEMICAL PROPERTIES

Appearance at 20°C and 101.3 kPa:	White crystalline powder at room temperature
Melting Point:	100-102°C
Specific Gravity:	1.25
Vapour Pressure:	4.48 × 10 ⁻⁵ Pa at 25°C
Water Solubility:	2.7 × 10 ⁻⁵ g/L at 20°C 1.01 mg/L (calculated (1))
Henry's constant	5.83 × 10 ⁻⁸ atm·m ³ /mole (calculated)
Partition Co-efficient (n-octanol/water) log P_{ow}:	5.00 at 21°C
Hydrolysis as a function of pH:	not applicable because of low water solubility. The notified chemical contains hydrolysable functional groups.
no	
Adsorption/Desorption:	not measured. The log K _{oc} of 2-BON can be estimated using the following formula: logK _{oc} = logK _{ow} - 0.21 (Dragun, 1988 (2)) logK _{oc} = 4.79
Dissociation Constant pK_a:	not applicable. 2-BON has no dissociable functionalities
Flash Point:	not flammable

Flammability Limits:	not flammable
Combustion Products:	Complete combustion products are carbon dioxide and water
Autoignition Temperature:	not flammable
Explosive Properties:	not explosive
Reactivity/Stability:	not expected to be reactive
Particle size:	> 100 µm

Comments of physico-chemical properties

The above comments provided by the notifier for omission of data are adequate. Most of the above results are supported by the US EPA's ASTER (Assessment Tools for the Evaluation of Risk) ecotoxicity profile (1) for the notified chemical. The exception is the ASTER water solubility value which is approximately two orders of magnitude higher than the water solubility value provided by the notifier.

The notified chemical's Henry constant value indicates that it is not volatile (1).

4. PURITY OF THE CHEMICAL

Degree of purity: 99.6% (99.2-100%)

Non-hazardous impurity:

Chemical name: 1,1-dibenzyl-2(1)-naphthalene
Weight percentage: ≤ 0.8%

Additive/Adjuvant: none

5. INDUSTRIAL USE

The notified chemical, in the form of a fine white powder, is to be used in the manufacture of heat sensitive paper, for use in facsimile machines and other devices.

6. OCCUPATIONAL EXPOSURE

Approximately 25 tonnes/annum of the chemical will be imported to Australia for the next 5 years. 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 60°C 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 not be sold directly to the public, but will be transported in 25 kg polyethylene lined bags to a single commercial customer site, where it is reformulated, and transferred to a paper coating machine for incorporation into paper, at a final concentration of 1.5% (dried). The paper is sized onto rolls and stored/sold to customers. The estimated total loss of 2-BON during manufacture of thermal paper is 100-200 kg/year, in the form of washings from mixing vessels and coating equipment. Solid waste will be disposed via the sewer.

The public may be exposed to thermal paper containing the chemical, however the chemical will be trapped within the paper matrix, at a final concentration of 1.5%, and human exposure would be minimal.

8. ENVIRONMENTAL EXPOSURE

. Release

Release at the reformulation site will occur during the washing of mixing vessels and coating equipment. The notifier claims that total losses of the notified chemical, through washing, would be 100 - 200 kg per year, based on an annual use of 25,000 kg of 2-BON. Assuming 20 batches per year, the amount of 2-BON released to the sewer per batch would be 5 - 10 kg. The site at Bayswater has an agreement in place with Melbourne Water for disposal via the sewer.

Thermal paper containing the notified chemical will ultimately be disposed of to landfill or will be incinerated. It is unlikely that 2-BON will leach from thermal paper as it is inextricably bound to the paper surface.

Releases to the environment may occur through processing of waste paper. This possibility is explored below.

. Fate

Limited environmental exposure of 2-BON will arise from the disposal of washings to sewer from the reformulation site. Based on the physico-chemical properties of the notified chemical it is expected to adsorb to suspended solids and organic matter present in the sewer and become associated with the sludge at the sewage treatment works. Aerobic biodegradation is likely to occur only slowly (see study below). Any 2-BON that enters receiving waters is likely to be negligible and become associated with the sediment.

Calculations using the Mackay level 1 environmental partitioning model indicates that 2-BON will partition predominantly into soil (~48%) and sediment (~45%), and to a lesser extent water (~6%). These results were obtained from the US EPA's ASTER database (1). It should be noted that the Mackay level 1 model is an equilibrium, steady state system, assuming no movement of the chemical between the various environmental compartments (eg air, water, soil, sediment) (3).

Unless incinerated, the notified chemical is likely to arrive in a dispersed manner in landfill bound to waste paper. As such, it will be immobile, and no leaching from landfill would be expected.

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 notifier has provided no data on the likely behaviour of the notified chemical during the recycling process. The notified 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 notified chemical will either

arrive in landfill where it can be expected to remain intact, or be destroyed through incineration.

- Biodegradation

A closed bottle test (OECD TG 301D) was undertaken to determine the biodegradability of 2-BON. Under the conditions of the study, only 7% of a 2 mg/L concentration of 2-BON had biodegraded after 28 days. Therefore, 2-BON is not readily biodegradable.

The ASTER ecotoxicity profile for 2-BON indicates that biodegradation half-life is likely to be greater than 100 days (1).

- Bioaccumulation

No bioaccumulation studies were provided. The notified chemical's log P_{ow} of 5.0, low water solubility and lack of ready biodegradability indicate it has the potential to bioaccumulate. The ASTER ecotoxicity profile for 2-BON has provided a calculated value for bioaccumulation in fish (1). The calculated bioconcentration factor of 3568 indicates that 2-BON is likely to accumulate in aquatic organisms.

Overall bioaccumulation in aquatic organisms is unlikely (from its proposed use) as exposure of aquatic environments to the notified chemical is expected to be negligible.

9. EVALUATION OF TOXICOLOGICAL DATA

9.1 Acute Toxicity

Table 1 Summary of the acute toxicity of [chemical name]

Test	Species	Outcome	Reference
Acute oral toxicity	Rat	LD ₅₀ > 5000 mg/kg	(4)
Acute dermal toxicity	Rat	LD ₅₀ > 2000 mg/kg	(5)
Skin Irritation	Rabbit	Non-irritant	(6)
Eye irritation	Rabbit	Non-irritant	(7)
Skin sensitisation	Guinea-pig	Non-sensitiser	(8)

9.1.1 Oral Toxicity (4)

In a preliminary study 2 male and 2 female CD rats were administered a gavage dose of 1000 mg/kg bw of 2-BON (50% w/v in 1% aqueous methylcellulose), and observed for 5 days. The LD₅₀ was estimated to be greater than 1000 mg/kg bw, on the basis of this study.

In the main study, 5 male and 5 female CD rats were administered a gavage dose of 5000 mg/kg bw of 2-BON (50% w/v in 1% aqueous methylcellulose), and observed for 14 days. There were no deaths. Pilo-erection occurred in all rats

within 5 minutes after dosing, and throughout the remainder of day 1. There were no other clinical signs, and recovery was complete by day 2. Bodyweight gains, and terminal autopsy findings were normal. It was concluded that the acute oral LD₅₀ of 2-BON was greater than 5000 mg/kg bw.

9.1.2 Dermal Toxicity (5)

5 male and 5 female CD rats were administered 2000 mg/kg bw of 2-BON (purity 99.6%), at a concentration of 60% w/v in distilled water, to shaved backskin under an occlusive dressing for 24 hours. All animals were observed for 14 days, and sacrificed and subjected to post-mortem macroscopic examination. There were no deaths, clinical signs of toxicity, or signs of dermal reaction at any application sites, and bodyweight gains were normal. It was concluded that the acute dermal LD₅₀ of 2-BON was greater than 2000 mg/kg bw.

9.1.3 Skin Irritation (6)

6 New Zealand White rabbits were administered 0.5 g of 2-BON (purity 99.6%), moistened with distilled water, to shaved, occluded backskin for 4 hours. After 4 hours the dressings were removed and the application site on each animal was washed with water to remove residual chemical. The treated skin was examined 30 minutes, and 2, 3 and 4 days after treatment. None of the animals showed any dermal response to treatment throughout the observation period. It was concluded that 2-BON was not a skin irritant.

9.1.4 Eye Irritation (7)

Approximately 75 mg of 2-BON (purity 99.6%) was instilled to the conjunctival sac of 1 eye of 6 NZ White rabbits. The eyes were examined after 1 hour, and 1, 2, 3, 4 and 7 days after instillation. No corneal damage or iridial inflammation was seen throughout the observation period. A diffuse crimson-red colouration of the conjunctivae was observed in 2 rabbits, 1 hour after instillation only. Mild conjunctival reactions were seen in the remaining animals. All conjunctival reactions had resolved 24 or 48 hours after instillation. 2-BON was a slight eye irritant.

9.1.5 Skin Sensitisation (8)

Skin sensitisation potential of 2-BON (purity 99.6%) was tested in 30 female albino Dunkin/Hartley guinea-pigs. A preliminary investigation showed that a maximum concentration of 50% w/w of 2-BON in alembicol (a product of coconut oil) could be applied topically for induction and challenge.

In the main study, induction was achieved by intradermal injections of 1% w/w of 2-BON in alembicol, followed after 1 week by topical application of 50% w/w of 2-BON in alembicol under an occlusive dressing for 48 hours. Control animals were treated similarly, with the exception of 2-BON from the intradermal injections and topical application. In the challenge phase, 2 weeks after induction, the test and control animals were topically administered 50% and 25% (different sites on each animal) for 48 hours under an occlusive dressing. The challenge sites were

evaluated 24, 48 and 72 hours after removal of the patches. There were no dermal reactions seen in any of the test or control animals. It was concluded that 2-BON did not cause delayed contact hypersensitivity in any of the animals.

9.2 Repeated Oral Dose Toxicity

9.2.1 28-day gavage study in rats (9)

Groups of 5 male and 5 female Charles River CD rats were dosed by oral gavage with 2-BON (0, 10, 100, 1000 mg/kg bw/d, 1% methylcellulose vehicle) for 28 days. Clinical signs, bodyweights, and food and water consumption were recorded. Haematology and biochemistry were performed prior to termination, in week 4. All animals underwent gross necropsy at termination, and microscopic examinations were performed on all control and high-dose rats.

There were no deaths. High-dose females, but not males, showed pilo-erection intermittently from day 5 onwards. Urea nitrogen was significantly lower in high-dose female rats only, but all other biochemical parameters were normal. Water consumption during week 2 showed a dose-related reduction, at all doses, which was most apparent in high-dose females. Bodyweight changes, food consumption, organ weights, haematology, and macroscopic and microscopic pathology were normal.

9.3 Genotoxicity

9.3.1 Salmonella typhimurium Reverse Mutation Assay (10)

In 2 separate bacterial mutagenicity tests, based on the test of Ames et al, 2-BON (purity 99.6%) was negative in *S. typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98 and TA 100, and *E. coli* strain WP2 *uvrA*, both in the presence and absence of S9. Positive controls indicated that the assay was performing satisfactorily.

9.3.2 Test for chromosomal aberrations in human lymphocytes *in vitro* (11)

The notified chemical, at concentrations of 12.5, 50 and 100 ug/mL, did not induce chromosomal aberrations in human lymphocytes *in vitro*. Positive controls indicated that the assay was performing satisfactorily.

9.4 Overall assessment of toxicological data

The acute oral toxicity of 2-BON was greater than 5000 mg/kg bw in rats, the acute dermal LD₅₀ was greater than 2000 mg/kg bw in rats, and the chemical was not a skin or eye irritant in rabbits, or a skin sensitiser in guinea pigs. An acute inhalation study was not submitted as the particles were not of a respirable diameter.

A 28-day oral gavage study in rats at dose levels of 0, 10, 100 or 1000 mg/kg bw/d showed a dose-related decrease in water consumption (all doses), and lower urea nitrogen levels in high-dose females. No other significant effects were observed.

2-BON would not be classified as hazardous according to Worksafe Australia's *Approved Criteria for Classifying Hazardous Substances* (12) in relation to Acute lethal effects (oral, dermal); Irritant effects (skin, eye), Sensitising effects (skin).

10. ASSESSMENT OF ENVIRONMENTAL EFFECTS

The following studies have been provided.

Test	Species	Result
Acute toxicity	Rainbow trout	96h LD ₅₀ > 0.69 mg/L NOEL ≥ 0.69 mg/L
Acute toxicity	<i>Daphnia magna</i>	48h LD ₅₀ > 0.41 mg/L NOEL ≥ 0.41 mg/L

The above studies were conducted according to OECD test guidelines. Results are based on measured concentrations. No mortalities were recorded in either study. 1.0 mg/L was the highest nominal test concentration that could be prepared due to the limited solubility of the test material in water. Since the test substance is chemically stable in water it is suspected that the apparent "loss" is due to settlement of insoluble material.

While, the above results indicate that 2-BON is non-toxic to the organisms tested up to the limit of its solubility care should be exercised in the interpretation of these results since it was observed that near nominal concentrations could not be maintained during the course of the study.

The ASTER ecotoxicity profile for 2-BON has provided calculated QSAR values for the acute and chronic toxicity to fish and aquatic invertebrates (see below).

Test	Species	Result
Acute toxicity	<i>Daphnia magna</i>	2d LC ₅₀ = 1.15 mg/L
Acute toxicity	Bluegill sunfish	4d LC ₅₀ = 1.51 mg/L
Acute toxicity	Fathead minnow	4d LC ₅₀ = 1.81 mg/L
Acute toxicity	Channel catfish	4d LC ₅₀ = 0.78 mg/L
Acute toxicity	Rainbow trout	4d LC ₅₀ = 0.67 mg/L
Chronic toxicity	Fathead minnow	32d MATC = 63 µg/L

The above results indicate that 2-BON is moderately toxic to aquatic invertebrates, is moderately to highly toxic to fish under acute conditions and is very highly toxic under chronic conditions. The results of the QSARs analysis indicates that 2-BON contains functional moieties capable of toxic action to fish and aquatic invertebrates at relatively low concentrations (< 1 ppm). However, it should be noted that the concentrations at which these toxic effects were calculated are above the water solubility value of 2-BON as provided by the notifier. Therefore, the limited solubility of 2-BON in water and removal to sediments is expected to

attenuate in the field the theoretical toxic effects that were demonstrated by the QSAR analysis.

11. ASSESSMENT OF ENVIRONMENTAL HAZARD

Environmental exposure to 2-BON will occur when waste from the reformulation site is disposed to sewer. The amount of 2-BON released to the sewer per batch would be 5 - 10 kg. Assuming a flow of 500 ML/day at the sewerage treatment plant the concentration of 2-BON would be ~20 ppb. Further dilution in the order of 1:5 - 1:25 would be expected in the receiving waters. Therefore, the estimated environmental concentration of 2-BON from the proposed use is at a level that is not expected to present a significant hazard to the environment. The above calculation assumes no degradation or adsorption of 2-BON in the sewer or the receiving waters.

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

12. ASSESSMENT OF PUBLIC AND OCCUPATIONAL HEALTH AND SAFETY EFFECTS

2-BON is expected to exhibit low oral and dermal toxicity and be non irritating to skin and slightly to eyes. It is not expected to be a sensitising agent, nor to exhibit significant toxicity following repeated or prolonged exposure and is not expected to be genotoxic.

Occupational exposure to 2-BON 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 and eye irritation.

Although significant public contact to 2-BON is expected to occur as a result of using treated products, exposure levels will be low since 2-BON 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 (2-BON) the following guidelines and precautions should be observed:

- . if engineering controls and work practices 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) (13) chemical type goggles (AS 1336, AS 1337) (14,15), rubber gloves (AS 2161) (16) overalls (AS 2919) (17) and protective shoes (AS/NZS 2210) (18) should be worn.
- . . good work practices 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 2-BON 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 (2-BON) was provided in Worksafe Australia format (19).

This MSDS was provided by Robert Bryce and Company Ltd as part of their notification statement. The accuracy of this information remains the responsibility of Robert Bryce and Company Ltd.

15. REQUIREMENTS FOR SECONDARY NOTIFICATION

Under the *Industrial Chemicals (Notification and Assessment) Act 1989*, secondary notification of 2-(phenylmethoxy) naphthalene (2-BON) shall be required if any of the circumstances stipulated under subsection 64(2) of the Act arise.

Should uses be proposed leading to greater exposure to the aquatic compartment, a secondary notification should be submitted, including results on algae and bioaccumulation to allow a re-assessment of the environmental hazard.

No other specific conditions are prescribed.

16. REFERENCES

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19. National Occupational Health and Safety Commission 1990, *Guidance Note for Completion of a Material Safety Data Sheet 2nd Edition*¹, Australian Government Publishing Services, Canberra, Australia.

¹ This guidance note, to which an MSDS must conform in accordance with the Act, has been superseded by the National Code of Practice for the Preparation of Material Safety Data Sheets [NOHSC:2011(1994)]