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May 2018

NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

PUBLIC REPORT

1,3-Dioxolane-4-methanol, 2-methyl-2-(2-methylpropyl)-

This Assessment has been compiled in accordance with the provisions of the *Industrial Chemicals (Notification and Assessment) Act 1989* (the Act) and Regulations. This legislation is an Act of the Commonwealth of Australia. The National Industrial Chemicals Notification and Assessment Scheme (NICNAS) is administered by the Department of Health, and conducts the risk assessment for public health and occupational health and safety. The assessment of environmental risk is conducted by the Department of the Environment and Energy.

This Public Report is available for viewing and downloading from the NICNAS website or available on request, free of charge, by contacting NICNAS. For requests and enquiries please contact the NICNAS Administration Coordinator at:

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Director
NICNAS

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SUMMARY

The following details will be published in the NICNAS *Chemical Gazette:*

ASSESSMENT REFERENCE	APPLICANT(S)	CHEMICAL OR TRADE NAME	HAZARDOUS CHEMICAL	INTRODUCTION VOLUME	USE
STD/1604	Solvay Interox Pty Ltd	1,3-Dioxolane-4-methanol, 2-methyl-2-(2-methylpropyl)-	Yes	≤ 10 tonnes per annum	Component of fluids used in oil/gas operations

CONCLUSIONS AND REGULATORY OBLIGATIONS

Hazard classification
Based on the available information, the notified chemical is recommended for hazard classification according to the *Globally Harmonised System of Classification and Labelling of Chemicals (GHS)*, as adopted for industrial chemicals in Australia. The recommended hazard classification is presented in the following table.

Hazard classification	*Hazard statement*
Serious eye damage/irreversible effects on the eye (Category 1)	H318 - Causes serious eye damage

Human health risk assessment
Provided that the recommended controls are being adhered to, under the conditions of the occupational settings described, the notified chemical is not considered to pose an unreasonable risk to the health of workers.

When used in the proposed manner, the notified chemical is not considered to pose an unreasonable risk to public health.

Environmental risk assessment
On the basis of the PEC/PNEC ratio and the reported use pattern, the notified chemical is not considered to pose an unreasonable risk to the environment.

Recommendations

REGULATORY CONTROLS

Hazard Classification and Labelling

- The notified chemical should be classified as follows:
  - Serious eye damage/irreversible effects on the eye (Category 1): H318 - Causes serious eye damage

The above should be used for products/mixtures containing the notified chemical, if applicable, based on the concentration of the notified chemical present and the intended use/exposure scenario.

CONTROL MEASURES

Occupational Health and Safety

- A person conducting a business or undertaking at a workplace should implement the following engineering controls to minimise occupational exposure to the notified chemical as introduced:
  - Closed mixing/pumping systems

- A person conducting a business or undertaking at a workplace should implement the following safe work practices to minimise occupational exposure during handling of the notified chemical:
  - Avoid contact with eyes

- A person conducting a business or undertaking at a workplace should ensure that the following personal protective equipment is used by workers to minimise occupational exposure to the notified chemical:
  - Protective goggles

  Guidance in selection of personal protective equipment can be obtained from Australian, Australian/New Zealand or other approved standards.

- A copy of the SDS should be easily accessible to employees.

- If products and mixtures containing the notified chemical are classified as hazardous to health in accordance with the *Globally Harmonised System of Classification and Labelling of Chemicals (GHS)* as adopted for industrial chemicals in Australia, workplace practices and control procedures consistent with provisions of State and Territory hazardous substances legislation should be in operation.

Disposal

- Where reuse or recycling are not appropriate, dispose of the notified chemical in an environmentally sound manner in accordance with relevant Commonwealth, state, territory and local government legislation.

Storage

- The handling and storage of the notified chemical should be in accordance with the Safe Work Australia Code of Practice for *Managing Risks of Hazardous Chemicals in the Workplace* (SWA, 2012) or relevant State or Territory Code of Practice.

Emergency procedures

- Spills or accidental release of the notified chemical should be handled by physical containment, collection and subsequent disposal.

Regulatory Obligations

Secondary Notification
This risk assessment is based on the information available at the time of notification. The Director may call for the reassessment of the chemical under secondary notification provisions based on changes in certain circumstances. Under Section 64 of the *Industrial Chemicals (Notification and Assessment) Act (1989)* the notifier, as well as any other importer or manufacturer of the notified chemical, have post-assessment regulatory obligations to notify NICNAS when any of these circumstances change. These obligations apply even when the notified chemical is listed on the Australian Inventory of Chemical Substances (AICS).

Therefore, the Director of NICNAS must be notified in writing within 28 days by the notifier, other importer or manufacturer:

(1) Under Section 64(1) of the Act; if
  - the chemical is intended to be used in oil/gas operations involving hydraulic fracturing;

or

(2) Under Section 64(2) of the Act; if
  - the function or use of the chemical has changed from a component of fluids used in oil/gas operations, or is likely to change significantly;
  - the amount of chemical being introduced has increased, or is likely to increase, significantly;
  - the chemical has begun to be manufactured in Australia;
  - additional information has become available to the person as to an adverse effect of the chemical on occupational health and safety, public health, or the environment.

The Director will then decide whether a reassessment (i.e. a secondary notification and assessment) is required.

Safety Data Sheet

The SDS of the product containing the notified chemical provided by the notifier was reviewed by NICNAS. The accuracy of the information on the SDS remains the responsibility of the applicant.

ASSESSMENT DETAILS

This notification has been conducted under the cooperative arrangement with Canada. The health and environmental hazard assessment components of the Canadian report were provided to NICNAS and, where appropriate, used in this assessment report. The other elements of the risk assessment and recommendations on safe use of the notified chemical were carried out by NICNAS.

1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT
Solvay Interox Pty Ltd (ABN: 70 000 882 137)
20-22 McPherson Street
BANKSMEADOW NSW 2019

NOTIFICATION CATEGORY
Standard (Reduced fee notification): Chemical other than polymer (more than 1 tonne per year) – Approved foreign scheme – Canada

EXEMPT INFORMATION (SECTION 75 OF THE ACT)
Data items and details claimed exempt from publication: other names, analytical data, degree of purity, impurities, use details and import volume

VARIATION OF DATA REQUIREMENTS (SECTION 24 OF THE ACT)
Variation to the schedule of data requirements is claimed as follows: dissociation constant, flammability limits, explosive properties, oxidising properties and repeated dose toxicity

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)
None

NOTIFICATION IN OTHER COUNTRIES
Canada (2016)
EU (2016)
USA (2016)

2. IDENTITY OF CHEMICAL

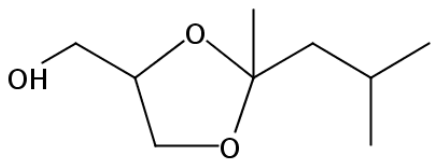
MARKETING NAME
1,3-Dioxolane-4-methanol, 2-methyl-2-(2-methylpropyl)-

CAS NUMBER
5660-53-7

CHEMICAL NAME
1,3-Dioxolane-4-methanol, 2-methyl-2-(2-methylpropyl)-

MOLECULAR FORMULA
$C_9H_{18}O_3$

STRUCTURAL FORMULA



MOLECULAR WEIGHT
174.24 Da

ANALYTICAL DATA
Reference NMR, IR, UV and GC-MS spectra were provided.

3. COMPOSITION

DEGREE OF PURITY
> 98%

4. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE AT 20 °C AND 101.3 kPa: Liquid

Property	Value	Data Source/Justification
Melting Point	< -50 °C	Measured
Boiling Point	230.5 °C	Measured
Density	1,001 kg/m^3 at 20 °C	Measured
Vapour Pressure	88.4 × 10^{-3} kPa at 20 °C	Measured
Water Solubility	34.6 g/L at 20 °C	Measured
Hydrolysis as a Function of pH	$t_{½}$ = 17.45 h at pH 4, 20 °C. No hydrolysis occurred at pH 7 and 9.	Measured
Partition Coefficient (n-octanol/water)	log P_{OW} = 1.6 at 20 °C	Measured
Adsorption/Desorption	log K_{oc} = 1.36	Measured
Dissociation Constant	Not determined	Contains no functional groups that are expected to dissociate under environmental conditions
Flash Point	113 °C at 101.3 kPa	Measured
Flammability	Combustible liquid*	Based on flash point
Autoignition Temperature	360 °C	Measured
Explosive Properties	Not determined	Contains no functional groups that would imply explosive properties
Oxidising Properties	Not determined	Contains no functional groups that would imply oxidative properties

* Based on *Australian Standard AS1940* definitions

DISCUSSION OF PROPERTIES
For full details of tests on physical and chemical properties that were not assessed in Canada, refer to Appendix A.

Reactivity
The notified chemical is expected to be stable under normal conditions of use. Some hydrolysis may be observed under low pH conditions.

Physical hazard classification
Based on the submitted physico-chemical data depicted in the above table, the notified chemical is not recommended for hazard classification according to the *Globally Harmonised System of Classification and Labelling of Chemicals (GHS)*, as adopted for industrial chemicals in Australia.

The notified chemical has a flash point of 113 °C. Based on *Australian Standard AS1940* definitions for combustible liquids, a liquid that has a flash point of 150 °C or less is a Class C1 combustible liquid.

5. INTRODUCTION AND USE INFORMATION

MODE OF INTRODUCTION OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS
The notified chemical will not be manufactured in Australia. It will be imported as a neat chemical or in a formulation at a concentration ≤ 50%.

MAXIMUM INTRODUCTION VOLUME OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS

Year	*1*	*2*	*3*	*4*	*5*
Tonnes	1-10	1-10	1-10	1-10	1-10

PORT OF ENTRY
Sydney, Melbourne, Brisbane and Perth

TRANSPORTATION AND PACKAGING
The notified chemical will be imported in 205 L HDPE drums and transported in the original containers by road or railway in its neat form or in a formulation at a concentration ≤ 50%.

USE
The notified chemical will be used as a component of fluids used in oil/gas well operations at an end-use concentration of < 5%.

OPERATION DESCRIPTION
No reformulation or repackaging of the notified chemical will occur in Australia. The notified chemical in neat form or the formulation containing the notified chemical at ≤ 50% concentration will be used at the oil/gas drilling sites. Workers will open the 205 L drums containing the neat notified chemical or the formulation and connect the pumping equipment to the drums. The contents will be transferred and mixed with other components in an on-site holding tank. Once the process is completed, the pumping equipment will be disconnected. The final fluid containing the notified chemical at ≤ 5% concentration will be injected into the well from the holding tank. For off-shore operations, when the well treatment is completed the fluid will be pumped back out and stored in pits on the rig. The recovered water phase may be re-injected into the reservoir for pressure maintenance or it may be further diluted and discharged into the ocean in batch mode. When used for on-shore operations, the retrieved fluid will be collected and sent to on-site treatment and water recycling process.

6. HUMAN HEALTH IMPLICATIONS

6.1. Exposure Assessment

6.1.1. Occupational Exposure

CATEGORY OF WORKERS

Category of Worker	*Exposure Duration (hours/day)*	*Exposure Frequency (days/year)*
Transport and storage	1-8	20
Oil and gas rig workers	2-4	20-40

EXPOSURE DETAILS
Transport and Storage
Transport and storage workers may come into contact with the notified chemical in neat form or in a formulation at a concentration ≤ 50%, only in the event of accidental breaches of the containers.

End Use
During well treatment, dermal or ocular exposure to the notified chemical at up to 100% concentration may occur due to possible spills and splashes in transfer, mixing and pumping processes. After the well treatment, the fluid containing the notified chemical will be pumped back to the surface and workers involved in the operations may continually have potential for dermal or ocular exposure to the notified chemical at ≤ 5% concentration. The exposure is expected to be minimised by the use of quick connect fittings, closed mixing/pumping systems, and personal protective equipment (PPE) including gloves, goggles and coveralls. Inhalation exposure is not expected under normal use conditions unless aerosols, vapours or mists are formed during use. The notified chemical and mixtures containing the notified chemical will be used in open areas in the oil/gas fields where accumulation of aerosols, vapours or mists is not expected to be significant.

6.1.2. Public Exposure
The notified chemical will not be used by the public. It will only be used for industrial applications in remote oil/gas fields where public access will be very limited. Therefore public exposure to the notified chemical is not expected under normal use conditions.

6.2. Human Health Effects Assessment

The results from toxicological investigations conducted on the notified chemical and a structurally similar analogue (1,3-Dioxolane-4-methanol, 2,2-dimethyl-, CAS RN 100-79-8) are summarised in the following table. For full details of the acute inhalation study that was not assessed in Canada, refer to Appendix B.

Endpoint	*Result and Assessment Conclusion*	*Test Substance*	*Test Method*
Rat, acute oral toxicity	LD50 > 2,000 mg/kg bw; low toxicity	Notified chemical	OECD TG 423
Rat, acute dermal toxicity	LD50 > 2,000 mg/kg bw; low toxicity	Analogue	OECD TG 402
Rat, acute inhalation toxicity*	LC50 > 5.11 mg/L/4 hour; low toxicity	Analogue	OECD TG 403
Rabbit, skin irritation	non-irritating	Notified chemical	OECD TG 404
Rabbit, eye irritation	corrosive	Notified chemical	OECD TG 405
Guinea pig, skin sensitisation – non-adjuvant test	no evidence of sensitisation	Notified chemical	OECD TG 406
Rat, combined repeat dose oral toxicity with reproduction / developmental toxicity screening test – 42 days for females	Systemic NOAEL = 1,000 mg/kg bw/day Reproductive NOEL > 1,000 mg/kg bw/day	Analogue	OECD TG 422
Mutagenicity – bacterial reverse mutation	non mutagenic	Notified chemical	OECD TG 471
Genotoxicity – *in vitro* chromosome aberration	non genotoxic	Notified chemical	OECD TG 473
Genotoxicity – *in vivo* mouse micronucleus assay	non genotoxic	Analogue	OECD TG 474

* Not assessed in Canada

Toxicokinetics, metabolism and distribution

No information on *in vivo* toxicokinetics, metabolism and distribution was submitted for the notified chemical. Based on the low molecular weight (174.24 Da) and a log Pow of 1.6, the notified chemical is expected to be readily absorbed through biomembranes including skin upon intake and distributed *in vivo* via body fluid circulations.

Acute toxicity

Acute oral toxicity of the notified chemical was tested on female Wistar rats. Two groups of three animals each received the notified chemical by oral gavage at a dose of 300 mg/kg bw and another two groups of three animals each received the notified chemical at a dose of 2,000 mg/kg bw. No deaths occurred and no signs of systemic toxicity were observed. Clinical signs for animals treated at 2,000 mg/kg bw included prostration, ataxia, salivation and dyspnoea. Congestion and multifocal pale areas of the liver and congestion of the lungs were noted at macroscopic examination of animals in both dose groups. The study authors concluded that the notified chemical showed low acute oral toxicity with an LD50 > 2,000 mg/kg bw.

Acute dermal toxicity of the analogue was tested on male and female Sprague Dawley rats. Animals received a single application of 2,000 mg/kg bw under a semi-occlusive dressing for 24 hours. No deaths occurred and no signs of systemic toxicity were observed. On the application site, two females presented scabs and a very slight erythema was noted in one of these two females. The analogue showed low acute dermal toxicity with an LD50 > 2,000 mg/kg bw.

Acute inhalation toxicity of the analogue was tested on male and female Wistar rats (Appendix B.1). The analogue showed low acute inhalation toxicity with an LC50 > 5.11 mg/L/4 hour.

Irritation and sensitisation

A primary skin irritation study was conducted with the notified chemical on male New Zealand White rabbits. The undiluted notified chemical (0.5 mL) was applied to the skin and held in place with a gauze patch for 4 hours. No deaths occurred and no clinical signs of systemic toxicity were observed. The notified chemical did

not elicit any skin reactions. The notified chemical was not considered by the study authors to be a dermal irritant under the conditions of the study.

A primary eye irritation study was conducted with the notified chemical on male New Zealand White rabbits. The undiluted notified chemical (0.1 mL) was placed into the lower conjunctival sac of one eye while the other eye served as control. No deaths occurred and no evidence of systemic toxicity was observed. Opacity, conjunctivae redness, chemosis and iritis were observed in animals from 1 hour up to 48 hours post treatment. At 48 hours, corneal ulceration, considered an irreversible lesion, was observed. The notified chemical was considered by the study authors to be corrosive under the conditions of this study.

The notified chemical was evaluated for skin sensitisation using the Buehler method in the guinea pig. In the induction phase, 20 test animals received an application of the undiluted notified chemical to the left flank under an occlusive dressing for 6 hours on days 0, 7, and 15. On day 27, animals were challenged by receiving an application of the undiluted notified chemical to the left flank under an occlusive dressing for 6 hours. Skin reactions were noted at 24 and 48 hours after patch removal during induction phase. One animal died during the induction phase; however, the death was not considered to be treatment related. Following challenge, no skin reactions were noted at 24 or 48 hours. The notified chemical was not considered by the study authors to be a skin sensitiser under the conditions of the assay.

Repeated dose toxicity
A combined oral repeated dose and reproductive and developmental toxicity study was conducted with the analogue on Sprague-Dawley rats. The animals received the analogue by oral gavage at a dose of 250, 500 or 1,000 mg/kg bw/day. Males were exposed 2 days before pairing, during pairing (5 days) and up to terminal sacrifice for a total of 40 days. Females were exposed 2 weeks prior to pairing, during pairing (up to 5 days), gestation and lactation, and up to 5 days postpartum for a total of 42 days.

One female given 1,000 mg/kg bw/day was prematurely sacrificed on day 4 *post coitus* on ethical grounds as this animal displayed hind limb paralysis before sacrifice. No necropsy findings were noted. In this animal, the most probable cause of clinical signs leading to premature sacrifice was considered to be early malignant lymphoma infiltrating the bone marrow (sternum) and the liver. Although the infiltrate in the bone marrow was slight in the sternum, higher severity in other locations, particularly the vertebrae, may have compressed the nerve tissue and induced hind limb paralysis. In view of the duration of the treatment and the absence of pre-neoplastic or neoplastic hematopoietic lesions in other treated animals, this isolated finding was considered by the study authors to be incidental.

When compared with controls, there was a slight increase in the mean absolute and relative liver weights in males given the analogue at 1,000 mg/kg bw/day, reaching statistical significance for the relative liver weight. A minimal trend was also present at 500 mg/kg bw/day, but the differences were not statistically significant. These variations were considered to be related to the analogue but were not considered to be adverse in view of the slight magnitude of the changes and lack of accompanying histopathological changes.

Treatment-related microscopic findings occurred in the kidneys of males given the analogue at 1,000 mg/kg bw/day. In the kidneys, tubular hyaline droplets were seen with increased incidence and severity. This was characterised by the presence of dense eosinophilic droplets in proximal tubular epithelium. Hyaline droplets, occasionally seen in untreated male rats, are consistent with the presence of α-2μ-globulin and are known to increase after treatment with a wide range of drugs or chemicals. The findings were not considered by the study authors to be relevant to humans.

There were no significant findings at 250 and 500 mg/kg bw/day for the analogue.

There were no analogue related findings for the following parameters: clinical signs, functional observational battery, food consumption, body weight or body weight gain, haematology, oestrus cycle and fertility. There were no effects on the mean numbers of *corpora lutea*, implantations or pups at any dose-level, nor on the duration of gestation or the extent of post-implantation losses. There were no effects on pup viability, body weight and body weight change in pups and on the percentage of male/female pups at birth at any dose-levels.

Given the experimental conditions of the study, 1,000 mg/kg bw/day was considered by the study authors to be the no observed adverse effect level (NOAEL) for parental and systemic toxicity based on findings in the livers of males. The no observed effect level (NOEL) for reproductive performance (mating and fertility) and for toxic

effects on progeny was considered by the study author to be greater than 1,000 mg/kg bw/day. The analogue showed low oral repeated dose toxicity and low reproductive/developmental toxicity.

Mutagenicity/Genotoxicity
The notified chemical was evaluated for *in vitro* mutagenicity in a bacterial reverse mutation assay at concentrations up to 5,000 µg/plate in both the presence and absence of metabolic activation (S9). Neither an increase in the number of revertant colonies nor a dose-related response was observed in five strains of *Salmonella typhimurium* (TA98, TA100, TA1535, TA1537 and TA102) either with or without metabolic activation. The notified chemical was considered by the study authors to be negative for *in vitro* mutagenicity under the conditions of the assay.

The notified chemical was tested for *in vitro* clastogenicity in a chromosomal aberration study using Chinese hamster ovary cells. In the first assay, cells were exposed to various concentrations of the notified chemical for 3 hours both in the presence and absence of metabolic activation (S9). In the second assay, cells were exposed to various concentrations of the notified chemical for 23 hours without S9. Cytotoxicity was noted for the continuous 23 hour exposure. In both experiments, no biologically or statistically significant increase in the number of cells carrying structural chromosome aberrations was observed. The notified chemical was considered by the study authors to be negative for *in vitro* clastogenicity under the conditions of the assay.

The analogue was tested for *in vivo* clastogenicity in a mouse micronucleus assay. Swiss male mice received the analogue by intraperitoneal administration at a dose of 2,000 mg/kg bw. Animals were treated twice at 0 and 24 h (2 treatments at 24 hours interval) and sampled approximately 24 hours following the final treatment. There were no statistically significant or biologically relevant increases in the frequency of detected micronuclei following administration. The analogue was considered by the study authors to be negative for *in vivo* clastogenicity under the conditions of the assay.

Health hazard classification
Based on the available information, the notified chemical is recommended for hazard classification according to the *Globally Harmonised System of Classification and Labelling of Chemicals (GHS)*, as adopted for industrial chemicals in Australia. The recommended hazard classification is presented in the following table.

Hazard classification	*Hazard statement*
Serious eye damage/irreversible effects on the eye (Category 1)	H318 - Causes serious eye damage

6.3. Human Health Risk Characterisation

6.3.1. Occupational Health and Safety
The notified chemical is considered to be corrosive to the eyes. Workers may come into contact with the notified chemical at up to 100% concentration during well treatment. The expected use of closed mixing/pumping systems and PPE, including protective goggles, should minimise the risk of serious eye damage.

Provided that control measures are in place to minimise worker exposure to the notified chemical, the risk to the health of workers from use of the notified chemical is not considered to be unreasonable.

6.3.2. Public Health
Public exposure to the notified chemical is not expected under normal use conditions. Therefore, when used in the proposed manner, the notified chemical is not considered to pose an unreasonable risk to public health.

7. ENVIRONMENTAL IMPLICATIONS

7.1. Environmental Exposure & Fate Assessment

7.1.1. Environmental Exposure

RELEASE OF CHEMICAL AT SITE
The notified chemical will be imported as a neat chemical or in a formulation at a concentration ≤ 50% for use in off-shore drilling operations in Australia. The contents of the containers will be pumped to an on-site holding tank via the pumping equipment at the well site. The notified chemical will be mixed with other fluids resulting in end-use concentration of 5.0%, and will be pumped into the well using a closed system. Therefore, release of the notified chemical to the environment during import, storage, transport and blending processes should be

minimal. Spills or accidental release of the products containing the notified chemical are expected to be collected and disposed of by licensed waste management services in accordance with local government regulations.

RELEASE OF CHEMICAL FROM USE

All drilling will be conducted off-shore and a single drilling operation is expected to last 15 days. A spacer fluid containing the notified chemical at the concentration of 5% will be pumped into the well in order to displace the drilling fluid, and to clean the well prior to the cementing process. The cementing solution is then pumped into the well, lining the well and displacing the spacer fluid containing the notified chemical. The fluid containing the notified chemical is expected to be diluted 10-fold and stored in pits on the rig after the well treatment has been completed. This fluid may be reinjected into the reservoir for pressure maintenance or it will be further diluted and then discharged into the ocean in batch mode.

RELEASE OF CHEMICAL FROM DISPOSAL

The empty containers are expected to be recycled or disposed of to landfill on the shore. Waste, wash water and residues of the notified chemical in empty containers will be collected and released to on-site waste water treatment plant.

7.1.2. Environmental Fate

Based on the results of a biodegradability study provided by the notifier, the notified chemical is not readily biodegradable (1.9% biodegradation over 28 days). For the details of the environmental fate studies please refer to Appendix C. The notified chemical contains hydrolysable functionalities that are expected to hydrolyse rapidly under acidic condition ($t_{½}$ < 1 day). However, the notified chemical is not expected to hydrolyse under neutral or basic pH. The notified chemical is expected to remain in the water column due to high water solubility, persistence and low potential to adsorb to solid surfaces (log K_{oc} = 1.36). In addition, the notified chemical has low potential to bioaccumulate based on its low octanol-water partition coefficient value.

The half-life of the notified chemical in air is calculated to be 4.70 h based on reactions with hydroxyl radicals (AOPWIN v1.92, US EPA 2011). Therefore, in the event of release to the atmosphere, the notified chemical is not expected to persist in the atmospheric compartment.

The notified chemical disposed of to water systems is expected to disperse and ultimately degrade via biotic and abiotic pathways to form water and oxides of carbon.

7.1.3. Predicted Environmental Concentration (PEC)

As direct discharge of the notified chemical into seawater is likely from offshore use, the predicted environmental concentration (PEC) in seawater has been calculated based on the CHARM model (Thatcher et al., 2005). Based on the CHARM model, discharges of the spacer fluid and mixwater have been identified as the main routes for the notified chemical release. Mixwater will be discharged in batches and the greatest effect will occur within a radius (r) of 500 m from the discharge line. As the notified chemical is estimated to be diluted 10-fold in the pit before disposal into ocean in batch mode, the concentration of the notified chemical in the pit is expected to be 0.5%. Therefore, the PEC of the notified chemical in the water column due to mixwater discharge is calculated using the following equation:

$$PEC_{water} = C_{i,mixwater} \times D_{batch,mixwater}$$

In this relationship,

PEC_{water} = predicted environmental concentration in the water column (mg/L);

C_i = initial concentration of the notified chemical in mix water (mg/L);

$D_{batch,mixwater}$ = batchwise dilution factor of mix water (-).

It is reasonable to assume a density of 1 kg/L for the mixwater. Therefore, the concentration for the notified chemical in mixwater is calculated to be 5 g/L. The default dilution factor is set at 2.2×10^{-5} in the CHARM model under the batchwise discharge scenario (Thatcher et al., 2005, p. 49).

The resulting PEC_{water} is calculated to be:

$$PEC_{water} = C_{i,mixwater} \times D_{batch,mixwater} = 5\ g/L \times 2.2 \times 10^{-5} = 11 \times 10^{-5}\ g/L = 110 \mu g/L$$

The $PEC_{sediment}$ for a batchwise discharge scenario is not calculated in the CHARM model because there is assumed to be insufficient time to allow the establishment of equilibrium between the high short-term levels of the notified chemical in the water column arising from batchwise release of fluid and the levels of the chemical in sediments near the discharge point. Furthermore, the notified chemical has low potential to adsorb to sediments based on low adsorption coefficient.

7.2. Environmental Effects Assessment

The results from ecotoxicological investigations conducted on the notified chemical are summarised in the table below. Details of these studies can be found in Appendix C.

Endpoint	*Result*	*Assessment Conclusion*
Fish Toxicity	96 h LC50 > 100.3 mg/L	Not harmful to fish
Daphnia Toxicity	48 h EC50 > 95 mg/L	Not harmful to aquatic invertebrates
Algal Toxicity	72 h EC50 = 598 mg/L	Not harmful to algae

Based on the endpoints for toxicity of the notified chemical to marine aquatic organisms, the notified chemical is not considered to be harmful to marine aquatic organisms under the *Globally Harmonised System of Classification and Labelling of Chemicals* (GHS) (United Nations, 2009). Therefore, the notified chemical is not formally classified under the GHS.

7.2.1. Predicted No-Effect Concentration

The predicted no-effect concentration (PNEC) for the notified chemical has been calculated and is presented in the table below. The PNEC is calculated based on the endpoint for the most sensitive species for the notified chemical (Daphnia 48 h EC50 > 95 mg/L) and an assessment factor of 100 has been used as acute toxicity endpoints for three trophic levels are available.

Predicted No-Effect Concentration (PNEC) for the Aquatic Compartment		
Daphnia 48 h EC50	> 95	mg/L
Assessment Factor	100	
Mitigation Factor	1.00	
PNEC:	> 950	µg/L

7.3. Environmental Risk Assessment

Risk Assessment	PEC µg/L	PNEC µg/L	Q
Q - Ocean	110	> 950	< 0.12

The risk quotient (Q = PEC/PNEC) for ocean environment is calculated to be < 1. Based on its low n-octanol/water partition coefficient, the notified chemical is not expected to bioaccumulate in aquatic organisms. On the basis of PEC/PNEC ratio and the assessed use pattern, the notified chemical is not considered to pose an unreasonable risk to the aquatic environment.

APPENDIX A: PHYSICAL AND CHEMICAL PROPERTIES

Water Solubility 34.6 g/L at 20 °C

Method OECD TG 105 Water Solubility.
Remarks Shake Flask Method.
Test Facility Wildlife International (2014a)

Partition Coefficient (n-octanol/water) log P_{OW} = 1.6 at 20 °C

Method OECD TG 117 Partition Coefficient.
Remarks HPLC Method.
Test Facility Opus (2013)

Hydrolysis as a Function of pH $t_{½}$=17.45 h at pH=4, 20 °C. No hydrolysis occurred at pH 7 and 9.

Method OECD TG 111 Hydrolysis as a Function of pH.
EC Council Regulation No 440/2008 C.7 Degradation: Abiotic Degradation: Hydrolysis as a Function of pH.

pH	*T (°C)*	*$t_{½}$ (hours)*
4	20	17.45
4	37	3.06
4	50	1.10
7	50	No hydrolysis
9	50	No hydrolysis

Remarks No hydrolysis occurred at neutral or basic pH.
Test Facility Investigative Science Incorporated (2015)

Adsorption/Desorption – main test log K_{oc} = 1.36

Method OECD TG 106 Adsorption - Desorption Using a Batch Equilibrium Method.

Soil Type	*Organic Carbon Content (%)*	*pH*	*Koc (mL/g)*
Silty clay loam (3)	1.3	7.6	25.2
Loam (4)	3.0	6.9	17.0
Loamy sand (5)	0.9	7.5	38.4
Clay loam (6)	2.4	7.1	25.83
Loamy sand (7)	10.8	6.8	9.4

Remarks Tier 1 study was conducted to determine the soil/solution ratio (1:2) and the equilibrium time for adsorption (48 h) and the amount of adsorbed material on the surfaces of the test vessels.

Adsorption test
The air-dried soils were equilibrated with 0.01M $CaCl_2$ overnight with gentle shaker, and the test substance was added to give a starting concentration of about 750 mg/L. After 48 hours of agitation the samples were centrifuged at 5500 rpm for 10 min and an aqueous aliquot was taken for analysis by HPLC. The mean of the log Koc values for five soil types was reported. The notified chemical is considered highly mobile in all soils tested.
Test Facility Investigative Science Incorporated (2015)

Flash Point 113.0 °C at 101.325 kPa

Method EC Council Regulation No 440/2008 A.9 Flash Point.
Remarks Pensky-Martens closed tester method
Test Facility Wildlife International (2014b)

Autoignition Temperature 360 °C at 99.51 – 100.03 kPa

Method	EC Council Regulation No 440/2008 A.15 Auto-Ignition Temperature (Liquids and Gases)
Remarks	Commercially available auto-ignition temperature apparatus was used.
Test Facility	WIL Research (2014)

APPENDIX B: TOXICOLOGICAL INVESTIGATIONS

B.1. Acute toxicity – inhalation

TEST SUBSTANCE: Analogue

METHOD: OECD TG 403 Acute Inhalation Toxicity
EC Council Regulation No 440/2008, 93/21/EEC B.2 Acute Toxicity (Inhalation)

Species/Strain: Wistar Crl:WI
Vehicle: Dried compressed air
Method of Exposure: Nose-only exposure
Exposure Period: 4 hours
Physical Form: Aerosol

Particle Size

Group	*MMAD* (μm)*	*GSD* (μm)*	*Inhalable fraction (< 4 μm) (%)*
Sighting test	3.75	1.97	53.8
Main test	3.81	2.01	52.8

* MMAD: mass median aerodynamic diameters; GSD: geometric standard deviations

Remarks - Method: No significant deviations of protocol were noted.

A sighting test was performed at 5 mg/L target concentration for 4 hours on single animals of both sexes. Following the sighting test, the main test was also performed at 5 mg/L target concentration using five rats per sex with a subsequent observation period of 14 days.

RESULTS

Group	*Number and Sex of Animals*	*Concentration (mg/L)*		*Mortality*
		Nominal	*Actual*	
Sighting test	2 (1 per sex)	22.67	5.04	0/2
Main test	10 (5 per sex)	22.37	5.11	0/10

LC50: > 5.11 mg/L/4 hours
Signs of Toxicity: No mortality was noted during the sighting and main tests.

Slight to moderate laboured respiration was recorded in all animals together with red-brown staining and/or wet fur on Day 0. These observations were considered to be related to the restraint and exposure procedures, and were not considered by the study authors to be toxicologically significant. Each rat was symptom-free from Day 1.

In the sighting test, slight body weight loss was noted in both animals by Day 3. Both rats returned to their initial body weights by approximately Day 7. In the main test, slight body weight loss was also observed in 4 male and 2 female animals on Day 1. All affected animals normalised in the body weight by Day 3.

Effects in Organs: No internal or external findings were recorded at necropsy.
Remarks - Results: The test atmosphere concentrations were monitored in the breathing zone during the 4 hour exposure for 13 to 17 times at approximately equal intervals.

CONCLUSION: The notified chemical is of low toxicity via inhalation.

TEST FACILITY: CiToxLAB (2015)

APPENDIX C: ENVIRONMENTAL FATE AND ECOTOXICOLOGICAL INVESTIGATIONS

C.1. Environmental Fate

C.1.1. Ready biodegradability

TEST SUBSTANCE	Notified chemical
METHOD	OECD TG 310 Ready Biodegradability: CO_2 in sealed vessels (Headspace test)
Inoculum	Activated sludge
Exposure Period	28 days
Auxiliary Solvent	None
Analytical Monitoring	Total inorganic carbon (TIC)
Remarks - Method	A stock solution containing 2,000 mg carbon/L was prepared by adding 0.6459 g of the notified chemical into 200 ml of water and was diluted with test medium. The starting organic content of the solution was 20 mg/L. Biodegradation (mineralization to CO_2) was determined by measuring the net increase in total inorganic carbon levels over time.

RESULTS

Test substance		*Sodium Benzoate*	
Day	*% Degradation*	*Day*	*% Degradation*
8	0.10	8	82.30
14	0.68	14	86.90
21	0.66	21	93.44
28	1.93	28	93.79
35	1.79	35	95.43

Remarks - Results	The reference compound sodium benzoate reach the pass level of biodegradation by day 5 indicating the suitability of the inoculum. The toxicity control exceeded 25% biodegradation showing toxicity was not a factor inhibiting the biodegradability of the test substance.
CONCLUSION	The notified chemical is not readily biodegradable.
TEST FACILITY	Rhodia Poliamida & Especialidades Ltd (2007)

C.2. Ecotoxicological Investigations

C.2.1. Acute toxicity to fish

TEST SUBSTANCE	Notified chemical
METHOD	OECD TG 203 Fish, Acute Toxicity Test –Static.
Species	*Oncorhynchus mykiss* (rainbow trout)
Exposure Period	96 h
Auxiliary Solvent	None
Water Hardness	240 mg $CaCO_3$/L
Analytical Monitoring	HPLC
Remarks – Method	The test was conducted at a single concentration limit test (nominal concentration of 110 mg/L). Test solutions were prepared by adding 1.65 g of the notified chemical into 15 L of water and gently mixed for 1-2 min.

RESULTS

Concentration mg/L		*Number of Fish*	*Mortality*			
Nominal	*Actual (Time-Weighted Mean)*		*24 h*	*48 h*	*72 h*	*96 h*
Control	< MDL[a]	10	0	0	0	0

Concentration mg/L		*Number of Fish*	*Mortality*			
Nominal	*Actual (Time-Weighted Mean)*		*24 h*	*48 h*	*72 h*	*96 h*
Control	< MDL	10	0	0	0	0
Control	< MDL	10	0	0	0	0
Laboratory Control[b]	NM[c]	10	0	0	0	0
110	100	10	0	0	0	0
110	101	10	0	0	0	0
110	100	10	0	0	0	0

a: MDL = method detection limit (10 mg/L)
b: NM = Not Measured
c: Laboratory control hardness ~370 mg/L $CaCO_3$

LC50	> 100.3 mg/L at 96 hours.
Remarks – Results	All validity criteria for the test were satisfied. Potassium chloride was used as the reference toxicant in this study. Mortality and impairment of fish did not exceed 10% in the controls.

CONCLUSION The notified chemical is not considered to be harmful to fish.

TEST FACILITY AquaTox Testing & Consulting Inc. (2015)

C.2.2. Acute toxicity to aquatic invertebrates

TEST SUBSTANCE Notified chemical

METHOD OECD TG 202 Daphnia sp. Acute Immobilisation Test and Reproduction Test – Static.

Species	*Daphnia magna*
Exposure Period	48 hours
Auxiliary Solvent	None
Water Hardness	140 mg $CaCO_3$/L
Analytical Monitoring	GC/MS
Remarks - Method	A primary stock solution was prepared by mixing a 0.20 of notified chemical in 2,000 ml of dilution water to achieve a nominal concentration of 100 mg/L and was used to prepare test solutions at nominal concentrations of 6.3, 13, 25 and 50 mg/L.

RESULTS

Concentration (mg/L)		*Number of D. magna*	*Number Immobilised*	
Nominal	*Actual*		*24 h*	*48 h*
Control	< LOQ	20	0	0
6.3	6.2	20	0	0
13	13	20	0	0
25	26	20	0	0
50	50	20	0	0
100	95	20	0	0

LOQ = the limit of quantitation

LC50	> 95 mg/L at 48 hours
NOEC	95 mg/L at 48 hours
Remarks - Results	All validity criteria for the test were satisfied. The reference test was conducted using potassium dichromate and confirmed the sensitivity of the system. No immobile daphnids were observed during the test. Therefore, the EC50 values were estimated to be greater than the highest concentration tested.

CONCLUSION The notified chemical is not considered to be harmful to aquatic invertebrates.

TEST FACILITY Wildlife International (2014c)

C.2.3. Algal growth inhibition test

TEST SUBSTANCE Notified chemical

METHOD OECD TG 201 Alga, Growth Inhibition Test.

Species	*Pseudokirchneriella subcapitata*
Exposure Period	72 hours
Concentration Range	Nominal: 31, 63, 125, 250, 500, 1000 mg/L Actual: 31, 65, 140, 249, 489, 944 mg/L
Auxiliary Solvent	None
Water Hardness	Not reported
Analytical Monitoring	GC/MS
Remarks - Method	A primary stock solution was prepared by dissolving 1.004 g of the notified chemical in 1000 ml of freshwater medium, and this stock solution was used to prepare solutions at nominal concentrations.

RESULTS

Biomass		*Growth*	
EC50	*NOEC*	*EC50*	*NOEC*
mg/L at 72 h	*mg/L*	*mg/L at 72 h*	*mg/L*
219	140	598	140

Remarks - Results All validity criteria for the test were satisfied. Measured concentrations of the notified chemical ranged from 92 to 103% of nominal. The results of the study are based on mean measured concentrations.

CONCLUSION The notified chemical is not considered to be harmful to algae.

TEST FACILITY Wildlife International (2014d)

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