File No: LTD/1898

April 2016

NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

PUBLIC REPORT

1*H*-1,4,7-Triazonine, octahydro-1,4,7-trimethyl-

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.

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:

Street Address:	Level 7, 260 Elizabeth Street, SURRY HILLS NSW 2010, AUSTRALIA.
Postal Address:	GPO Box 58, SYDNEY NSW 2001, AUSTRALIA.
TEL:	+ 61 2 8577 8800
FAX:	+ 61 2 8577 8888
Website:	www.nicnas.gov.au

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
LTD/1898	Akzo Nobel Pty Ltd	1*H*-1,4,7-Triazonine, octahydro-1,4,7-trimethyl-	Yes	≤ 0.25 tonne per annum	Component of paints and coatings

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*
Flammable liquids (Category 4)	H227- Combustible liquid
Skin corrosion/irritation (Category 1)	H314 - Causes severe skin burns and eye damage

Based on the available information, the notified chemical is recommended for hazard classification according to the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004), with the following risk phrase:

R35: Causes severe burns

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:
  - Flammable liquids (Category 4): H227- Combustible liquid
  - Skin corrosion/irritation (Category 1): H314 - Causes severe skin burns and 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.

- Due to the flammable properties of the notified chemical, the notifier should consider their obligations under the Australian Dangerous Goods Code (NTC, 2015).

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 in the product:
  - Sufficient ventilation
  - Spray booths used for spray applications where possible

- 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 as introduced in the product:
  - Avoid contact with skin and eyes
  - Avoid inhaling aerosols or spray mists

- 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 as introduced in the product:
  - Protective clothing/coveralls
  - Impervious gloves
  - Eye protection
  - Respiratory protection during spray application

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

- Spray applications should be carried out in accordance with the Safe Work Australia Code of Practice for *Spray Painting and Powder Coating* (SWA, 2015) or relevant State or Territory Code of Practice.

- A copy of the (M)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.

Emergency procedures

- Spills or accidental release of the notified chemical should be handled by containment, physical collection and subsequent safe 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 importation volume exceeds one tonne per annum notified chemical;
- the concentration of the notified chemical exceeds or is intended to exceed 0.3% in paints or coatings;

or

(2) Under Section 64(2) of the Act; if
- the function or use of the chemical has changed from a component of paints and coatings, 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.

(Material) Safety Data Sheet
The (M)SDSs of products containing the notified chemical provided by the notifier were reviewed by NICNAS. The accuracy of the information on the (M)SDSs remains the responsibility of the applicant.

ASSESSMENT DETAILS

1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)
Akzo Nobel Pty Ltd (ABN: 59 000 119 424)
57 Barclay Road
DERRIMUT VIC 3030

NOTIFICATION CATEGORY
Limited-small volume: Chemical other than polymer (1 tonne or less per year)

EXEMPT INFORMATION (SECTION 75 OF THE ACT)
Data items and details claimed exempt from publication: analytical data, impurities/additives and use details

VARIATION OF DATA REQUIREMENTS (SECTION 24 OF THE ACT)
Variation to the schedule of data requirements is claimed as follows: hydrolysis as a function of pH, adsorption/desorption, dissociation constant and flammability.

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)
None

NOTIFICATION IN OTHER COUNTRIES
None

2. IDENTITY OF CHEMICAL

MARKETING NAME(S)
Dragon Ligand

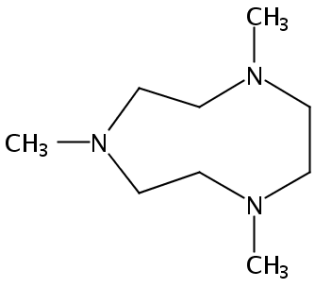
CAS NUMBER
96556-05-7

CHEMICAL NAME
1*H*-1,4,7-Triazonine, octahydro-1,4,7-trimethyl-

OTHER NAME(S)
1,4,7-Trimethyl-1,4,7-triazacyclononane
Me3TACN
MeTACN

MOLECULAR FORMULA
$C_9H_{21}N_3$

STRUCTURAL FORMULA



MOLECULAR WEIGHT
171.28 Da

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

3. COMPOSITION

DEGREE OF PURITY
> 95%

4. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE AT 20 °C AND 101.3 kPa: pale yellow liquid

Property	Value	Data Source/Justification
Melting Point/Freezing Point	< -20 °C	Measured
Boiling Point	207.3 °C at 101.4 kPa	Measured
Density	989 kg/m^3 at 20 °C	Measured
Vapour Pressure	0.123 kPa at 25 °C	Measured
Water Solubility	> 50 g/L at 20 °C	Measured
Hydrolysis as a Function of pH	$t_{½}$ > 1 year at pH 4, 7, and 9 at 25 °C	Measured (analogue chemical)
Partition Coefficient (n-octanol/water)	log Pow = 0.446 at pH 7	Measured
Surface Tension	59.8-67.5 mN/m at 20 °C	Measured
Adsorption/Desorption	log K_{oc} = 3.86 at 20 °C	Measured (analogue chemical)
Dissociation Constant	pKa = 8.63, 5.75, 2.86 (base)	Calculated using CompuDrug v3.6.2.1
Flash Point	69 °C at 100.9 kPa	Measured
Autoignition Temperature	200 °C	Measured
Explosive Properties	Predicted negative	Based on the chemical structure
Oxidising Properties	Predicted negative	Based on the chemical structure

DISCUSSION OF PROPERTIES
For full details of tests on physical and chemical properties, refer to Appendix A.

Reactivity
The notified chemical is expected to be stable under normal conditions of use.

Physical hazard classification
Based on the submitted physico-chemical data depicted in the above table, 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***
Flammable liquids (Category 4)	H227- 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 or reformulated in Australia. The notified chemical will be imported into Australia as a component of finished paints and coatings at ≤ 0.3% concentration.

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

Year	*1*	*2*	*3*	*4*	*5*
Tonnes	0.25	0.25	0.25	0.25	0.25

PORT OF ENTRY
Sydney, Melbourne, Brisbane, Perth and other ports

IDENTITY OF MANUFACTURER/RECIPIENTS
Akzo Nobel Pty Ltd

TRANSPORTATION AND PACKAGING
Finished paints and coatings containing the notified chemical at ≤ 0.3% concentration will be imported and transported in a range of containers, such as 5 L steel drums, up to 20 L polypropylene or metal cans (tin plate) or 200 L steel drums.

USE
The notified chemical will be used as a component (a drying agent to speed up the drying of paint) of paints and coatings by professionals and Do-It-Yourself (DIY) users in the yacht, marine and protective coating sectors, and in the decorative market.

OPERATION DESCRIPTION
The notified chemical will not be manufactured or reformulated in Australia. Imported paints and coatings will be repackaged into small containers and will be applied by brush, roller or spray onto a wide range of substrates by both professional and domestic users.

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 workers	1	5-10
Distribution and warehousing	1	5-10
Application process (end use) - sprayers	6	75
Application process (end use) - potmen	6	75

EXPOSURE DETAILS
Transport and storage workers are not expected to be exposed to the notified chemical (at ≤ 0.3% concentration) except in the unlikely event of an accident.

End-use
Exposure to paints and coatings containing the notified chemical (at ≤ 0.3% concentration) may occur during transfer, application and cleaning processes. The potential for exposure should be minimised through the stated use by the notifier of PPE (goggles, gloves and coveralls) by workers, including the use of respiratory protection during spray application. Inhalation exposure may be further mitigated through the use of exhaust ventilation and spray booths, where possible.

Workers may come into contact with substrates coated with the notified chemical after application. However, once the paints or coatings have dried, the notified chemical will be bound within a solid matrix and will not be available for exposure.

6.1.2. Public Exposure
Paints and coatings containing the notified chemical (at ≤ 0.3% concentration) will be available for use by DIY users. Exposure (dermal, ocular and inhalation) is expected to be on a less frequent basis than for professional users, although PPE may not be worn.

The public may come into contact with substrates coated with the notified chemical after application. However, once the paints or coatings have dried, the notified chemical will be bound within a solid matrix and will not be available for exposure.

6.2. Human Health Effects Assessment
No toxicity data were submitted.

The notified chemical has a low molecular weight (171.28 Da) and a log Pow of 0.446. Therefore, absorption across biological membranes is expected. However the high water solubility of the notified chemical may limit dermal absorption.

The pH of a water solution containing 1% notified chemical was measured to be 12.53 and hence the notified chemical is classified as Skin Corrosion/Irritation (Category 1): H314 - causes severe skin burns and eye damage. However, the notified chemical is expected to form a complex with a metal salt in end-use products to function as a drying catalyst, resulting in a significantly lower pH value of the product.

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*
Skin corrosion/irritation (Category 1)	H314 – Causes severe skin burns and eye damage

Based on the available information, the notified chemical is recommended for hazard classification according to the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004), with the following risk phrase:

R35: Causes severe burns

6.3. Human Health Risk Characterisation

6.3.1. Occupational Health and Safety
The notified chemical is classified as corrosive based on the pH value. However, the potential for causing corrosive effects is not expected in end-use products as the notified chemical is expected to form a complex with a metal salt in the formulation to significantly reduce the pH. In addition other components of the paint are expected to act as a buffer further reducing the pH. The low end-use concentration and expected control measures in place (e.g. PPE, sufficient ventilation and spray booths for spray painting booth) to minimise exposure should also reduce the risk of corrosive effects.

Once the paints and coatings have dried, the notified chemical will be bound within an inert matrix and will not be available for exposure.

Therefore, under the occupational settings described, the risk to the health of workers from use of the notified chemical is not considered to be unreasonable.

6.3.2. Public Health
There is potential for direct dermal, ocular and inhalation exposure of DIY users to the notified chemical at ≤ 0.3% concentration when paints and coatings containing the notified chemical are applied by brush, roller or spray. However, the frequency and extent of exposure is expected to be less than that of professional workers.

Members of the public may come into contact with surfaces coated with products containing the notified chemical. However, once the paints or coatings have dried, the notified chemical will be bound within the solid matrix and will not be available for exposure.

Based on the assessed use patterns, the risk to the public from use of the notified chemical is not considered to be unreasonable.

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 drying agent in finished paints and coating formulations for yacht, marine and protective applications, and will not be reformulated in Australia.

However, repackaging into containers of various sizes suitable for retail is expected to occur. There is unlikely to be any significant release to the environment from transport and storage, except in the case of accidental spills and leaks. In the event of spills, the products containing the notified chemical are expected to be collected with adsorbents, and disposed of to landfill in accordance with local government regulations.

The repackaging process will involve operations that will be highly automated, and is expected to occur within a fully enclosed environment. Therefore, significant release of the notified chemical from this process to the environment is not expected.

RELEASE OF CHEMICAL FROM USE
Products containing the notified chemical will be used by both professional and DIY users. During use, paints and coatings containing the notified chemical are expected to be applied by brush, roller and spray techniques. It is expected that some of the coating product will be in the form of overspray during spraying operations, and will typically entail disposal to landfill after being collected with adsorbents.

During use, the notified chemical may also be released to the environment as accidental spills and container residues. It is estimated by the notifier that up to 3% (or ≤ 7.5 kg of the import volume) may be released from accidental spill and container residues. These releases are expected to be collected and disposed of to landfill in accordance with local government regulations.

RELEASE OF CHEMICAL FROM DISPOSAL
The notified chemical in surface coatings is expected to share the fate of the substrate to which it has been applied, and are predominantly expected to be disposed to landfill, or thermally decomposed during metal reclamation.

Residues containing the notified chemical on brushes and rollers are expected to be rinsed into containers, and then allowed to cure before disposal as solid wastes to landfill. As a worst case scenario, it is assumed that up to 5% of the notified chemical used by DIY users may be incorrectly disposed of to the sewer, drains, or ground from waste and washing of application equipment.

7.1.2. Environmental Fate

No environmental fate data were submitted for the notified chemical. The majority of the notified chemical is expected to be cured within an inert coating matrix and is expected to share the fate of the articles to which it has been applied, which will involve eventual disposal to landfill, or undergo thermal decomposition during metal reclamation. The notified chemical is also expected to enter landfill as collected wastes and residues. Once cured, the notified chemical is not expected to be bioavailable.

An estimate of the biodegradability of the notified chemical has been calculated using BIOWIN v4.10 (US EPA, 2011). Based on its molecular structure, the notified chemical is not expected to be readily biodegradable. However, the notified chemical is not expected to be bioaccumulative, based on its high water solubility and low partition coefficient (log P_{OW} = 0.446). This is supported by the low bioconcentration factor (BCF = 3.16), calculated using BCFBAF v3.01 (US EPA, 2011). Based on its adsorption coefficient (log K_{OC} = 3.86), release to surface waters is unlikely to occur as partitioning to sludge and sediment is expected under environmental pH. In surface waters and in landfill, the notified chemical is expected to eventually degrade via biotic and abiotic processes to form water and oxides of carbon and nitrogen.

The notified chemical is moderately volatile from water based on its vapour pressure (0.123 kPa at 25 °C) and may slowly volatilise to air. The half-life of the notified chemical in air is calculated to be 28.96 min, based on reactions with hydroxyl radicals (AOPWIN v1.92; US EPA, 2011). Therefore, the notified chemical is not expected to persist in the air compartment.

7.1.3. Predicted Environmental Concentration (PEC)

The calculation for the predicted environmental concentration (PEC) is summarised in the table below. Based on the reported use in paints and coatings for professional and DIY-users, a conservative release of 5% to sewers on a nationwide basis over 365 days per year is used for the notified chemical. It is also assumes a worst case scenario where none of the notified chemical is removed during Sewage Treatment Plant (STP) processes.

Predicted Environmental Concentration (PEC) for the Aquatic Compartment		
Total Annual Import/Manufactured Volume	250	kg/year
Proportion expected to be released to sewer	5%	

Annual quantity of chemical released to sewer	12.5	kg/year
Days per year where release occurs	365	days/year
Daily chemical release:	0.03	kg/day
Water use	200.0	L/person/day
Population of Australia (Millions)	22.613	million
Removal within STP	0%	
Daily effluent production:	4,523	ML
Dilution Factor - River	1.0	
Dilution Factor - Ocean	10.0	
PEC - River:	0.008	µg/L
PEC - Ocean:	0.001	µg/L

STP effluent re-use for irrigation occurs throughout Australia. The agricultural irrigation application rate is assumed to be 1000 L/m^2/year (10 ML/ha/year). The notified chemical in this volume is assumed to infiltrate and accumulate in the top 10 cm of soil (density 1500 kg/m^3). Using these assumptions, irrigation with a concentration of 0.01 µg/L may potentially result in a soil concentration of approximately 0.05 µg/kg. Assuming accumulation of the notified chemical in soil for 5 and 10 years under repeated irrigation, the concentration of the notified chemical in the applied soil in 5 and 10 years may be approximately 0.25 µg/kg and 0.50 µg/kg, respectively.

7.2. Environmental Effects Assessment

No ecotoxicity data were submitted for the notified chemical. Ecotoxicological endpoints for the notified chemical were calculated based on ecological structure active relationship (ECOSAR v1.11; US EPA, 2012) equations. The acute and chronic endpoints are summarised in the table below.

Endpoint	*Result*	*Assessment Conclusion*
Acute Toxicity		
Fish Toxicity	96 h LC50 = 54.205 mg/L	Predicted to be harmful to fish (acute)
Daphnia Toxicity	48 h EC50 = 6.218 mg/L	Predicted to be toxic to aquatic invertebrates (acute)
Algal Toxicity	96 h EC50 = 5.535 mg/L	Predicted to be toxic to algae (acute)
Chronic Toxicity		
Fish Toxicity	ChV = 3.548 mg/L	Not predicted to be harmful to fish (chronic)
Daphnia Toxicity	ChV = 0.492 mg/L	Predicted to be toxic to aquatic invertebrates (chronic)
Algal Toxicity	ChV = 1.787 mg/L	Not predicted to be harmful to algae (chronic)

The notified chemical is predicted to be toxic to aquatic invertebrates and algae, and harmful to fish on an acute basis, and is predicted to be toxic to aquatic invertebrates on a chronic basis. The ECOSAR estimation procedure used here is a standard approach, and is considered reliable to provide general indications of the likely environmental effects of a chemical. However, this method is not considered sufficient to formally classify the acute and chronic hazards of the notified chemical to aquatic life under the Globally Harmonised System of Classification and Labelling of Chemicals (GHS) (United Nations, 2009).

7.2.1. Predicted No-Effect Concentration

The predicted no-effects concentration (PNEC) has been calculated from the most sensitive endpoint for *Daphnia*. A safety factor of 1000 was used given only modelled endpoints are available.

Predicted No-Effect Concentration (PNEC) for the Aquatic Compartment		
ChV (*Daphnia*, 21 d)	0.492	mg/L
Assessment Factor	1000	
Mitigation Factor	1.00	
PNEC:	0.492	µg/L

7.3. Environmental Risk Assessment

The Risk Quotients (Q = PEC/PNEC) have been calculated based on the predicted PEC and PNEC.

Risk Assessment	PEC µg/L	PNEC µg/L	Q
Q - River	0.008	0.492	**0.015**

Q - Ocean	0.001	0.492	**0.002**

The risk quotient for discharge of treated effluents containing the notified chemical to the aquatic environment indicates that the notified chemical is unlikely to reach ecotoxicologically significant concentrations in surface waters, based on its maximum annual importation quantity. Although the notified chemical is not predicted readily biodegradable, it is expected to have a low potential for bioaccumulation. On the basis of the PEC/PNEC ratio, maximum annual importation volume and assessed use pattern, the notified chemical is not expected to pose an unreasonable risk to the environment.

APPENDIX A: PHYSICAL AND CHEMICAL PROPERTIES

Melting Point/Freezing Point < -20 °C

Method OECD TG 102 Melting Point/Melting Range.
Remarks Measured by thermometer
Test Facility Harlan (2014a)

Boiling Point 207.3 ± 0.5 °C at 101.4 kPa

Method OECD TG 103 Boiling Point.
Remarks Determined by differential scanning calorimetry
Test Facility Harlan (2014a)

Density 898 kg/m^3 at 20 ± 0.5 °C

Method OECD TG 109 Density of Liquids and Solids.
Remarks A pycnometer method was used.
Test Facility Harlan (2014a)

Vapour Pressure 0.123 kPa at 25 °C

Method OECD TG 104 Vapour Pressure.
Remarks Determined using a vapour pressure balance
Test Facility Harlan (2014b)

Water Solubility > 50 g/L at 20 °C

Method OECD TG 105 Water Solubility.
EC Council Regulation No 440/2008 A.6 Water Solubility.
Remarks Flask Method
Test Facility Harlan (2014a)

Hydrolysis as a Function of pH $t_{½}$ > 1 year at pH 4, 7, and 9 at 25 °C

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

pH	*T (°C)*	*$t_{½}$ (years)*
4	25	> 1
7	25	> 1
9	25	> 1

Remarks After 5 days under the accelerated conditions of 50 °C, the rate of hydrolysis of the analogue chemical (dragon ligand chloride) was less than 10% at pH 4, 7, and 9. This equates to a half-life at 25 °C of $t_{½}$ > 1 year. Therefore, it can be concluded that under the conditions of the test the analogue chemical, and therefore the notified chemical, is expected to be hydrolytically stable.
Test Facility Huntingdon (1993)

Partition Coefficient (n-octanol/water) log Pow = 0.446 at pH 7

Method OECD TG 117 Partition Coefficient (n-octanol/water).
EC Council Regulation No 440/2008 A.8 Partition Coefficient.
Remarks HPLC Method
Test Facility Harlan (2014a)

Surface Tension 59.8-67.5 mN/m at 20 ± 0.5 °C

Method	OECD TG 115 Surface Tension of Aqueous Solutions.
Remarks	Concentration used: 1.028 g/L, 1.080 g/L and 1.015 g/L
Test Facility	Harlan (2014a)

Adsorption/Desorption – screening test log K_{oc} = 3.86 at 20 °C

Method	OECD TG 106 Adsorption - Desorption Using a Batch Equilibrium Method.
Remarks	Calculated for the analogue chemical (dragon ligand chloride) as the ratio between the concentration of the analogue in the soil phase and the concentration in the aqueous phase when adsorption equilibrium was reached.
Test Facility	Unilever (1994)

Dissociation Constant pKa = 8.63, 5.75, 2.86 (base) 7

Method	Calculated using CompuDrug v3.6.2.1.
Remarks	Calculated using the pKalc function of the PALLAS estimation software program.
Test Facility	Exponent International Ltd (2016)

Flash Point 69 ± 2 °C at 100.9 kPa

Method	EC Council Regulation No 440/2008 A.9 Flash Point.
Remarks	Closed cup
Test Facility	Harlan (2014c)

Autoignition Temperature 200 ± 5 °C

Method	EC Council Regulation No 440/2008 A.15 Auto-Ignition Temperature (Liquids and Gases).
Test Facility	Harlan (2014c)

Explosive Properties Predicted negative

Method	EC Council Regulation No 440/2008 A.14 Explosive Properties.
Remarks	Based on the chemical structure
Test Facility	Harlan (2014c)

Oxidizing Properties Predicted negative

Method	EC Council Regulation No 440/2008 A.21 Oxidizing Properties (Liquids).
Remarks	Based on the chemical structure
Test Facility	Harlan (2014c)

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