

# Qualitative Tier 2 Assessment

---

## N-Benzyl-Alkylpyridium Chloride

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterised by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.



## Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme<sup>1</sup> is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between “Dawson’s Bend” and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

N-benzyl-alkylpyridium chloride is a component in a water treatment product used to provide corrosion resistance from microbial influenced corrosion in the steel flowlines and spelines throughout the produced water management collection system. Process and usage information for this chemical is summarised in **Table 1**.

**Table 1 Water Management Facility Chemicals**

Chemical Name	CAS No.	Use	Percent Weight (%) in Product <sup>1</sup>
Benzyl-C-1-2-alkylpyridinium chloride	68909-18-2	Biocide	5

<sup>1</sup> Mid-point of range provided in SDS.

CAS No = Chemical Abstracts Service Number

The water treatment product could potentially be used for biocide treatment in FAPA but is currently not being used. Based on its use in other Santos project areas, dosage rates in water for this chemical in the biocide are in the range of  $1.0 \times 10^{-4}$  mg/L.

The assessment of toxicity of this chemical was used to develop initial screening criteria for human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. As detailed in the attachment and presented in **Table 2**, no data are available to derive toxicological reference and drinking water guideline values for n-benzyl-alkylpyridium chloride.

---

<sup>1</sup> Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).



**Table 2 Oral Reference Doses and Derived Drinking Water Guidelines**

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
N-benzyl-alkylpyridium chloride (68909-18-2)	- <sup>a</sup>	-	-	-	-	-

<sup>a</sup> – No data available.

CAS = Chemical Abstracts Service

mg/kg-day = milligram per kilogram-day

mg/L = milligram per litre

NOAEL = No observed adverse effect level

Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

**Table 3** present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5**, respectively. Refer to **Attachment 1** and the dossier regarding the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

**Table 3 PNECs Water – Tier 2 Chemicals**

Constituents	Endpoint	EC <sub>50</sub> or NOEC (mg/L)	Assessment Factor	PNEC <sub>water</sub> (mg/L)
N-benzyl-alkylpyridium chloride (68909-18-2)	Chronic <i>Daphnia</i> and algae	0.47	1000	0.0005

EC<sub>50</sub> = effects concentration – 50%

mg/L = milligram per litre

NOEC = no observable effects concentration

PNEC = predicted no effect concentration

Refer to **Attachment 1** for information on the development of PNECs listed above.



**Table 4 PNECs Sediment – Tier 2 Chemicals**

Constituents	Endpoint	EC <sub>50</sub> or NOEC (mg/kg wet wt)	Assessment Factor	PNEC <sub>sed</sub> (mg/kg wet wt)
N-benzyl-alkylpyridium chloride (68909-18-2)	a	-	-	0.007

<sup>a</sup>Calculated using equilibrium partitioning method.

EC<sub>50</sub> = effects concentration – 50%

mg/kg wet wt = milligram per kilogram wet weight

NOEC = no observable effects concentration

PNEC = predicted no effect concentration

Refer to **Attachment 1** for information on the development of PNECs listed above.

**Table 5 PNECs Soil – Tier 2 Chemicals**

Constituents	Endpoint	EC <sub>50</sub> or NOEC (mg/kg dry wt)	Assessment Factor	PNEC <sub>soil</sub> (mg/kg dry wt)
N-benzyl-alkylpyridium chloride (68909-18-2)	a	-	-	0.006

<sup>a</sup>Calculated using equilibrium partitioning method

EC<sub>50</sub> = effects concentration – 50%

mg/kg dry wt = milligram per kilogram dry weight

NOEC = no observable effects concentration

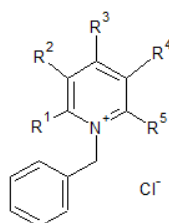
PNEC = predicted no effect concentration

Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

## General Overview

N-benzyl-alkylpyridium chloride is a mixture of alkyl pyridine quaternary ammonium salts. The molecular structure of n-benzyl-alkylpyridium chloride is presented in **Figure 1**. R1-5 are alkyl groups in the structure.



**Figure 1 Molecular Structure of N-Benzyl-Alkylpyridium Chloride <sup>2</sup>**

<sup>2</sup> Source <https://echa.europa.eu/registration-dossier/-/registered-dossier/21246/1>



N-benzyl-alkylpyridium chloride is inherently biodegradable. Components show variable sorption to soils and sediments. It is not expected to bioaccumulate based on the experimental octanol water partition coefficient ( $\log K_{ow}$ ).

The Persistent, Bioaccumulative and Toxic (PBT) assessment for n-benzyl-alkylpyridium chloride is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that n-benzyl-alkylpyridium chloride is not a PBT substance.

## Human Health Hazards

There is a low concern for human health hazards. Very little information exists regarding the specific hazards associated with n-benzyl alkylpyridium chloride. Thus, the information provided in this assessment was taken from data collected for quaternary ammonium compounds in general. Significant absorption of quaternary ammonium compounds is unlikely due to their highly ionic nature. As the substance is corrosive (i.e., pH=1.2), very little toxicity data are available with the exception of acute toxicity data showing a rat LD<sub>50</sub> of approximately 50 mg/kg-day<sup>3</sup>.

No data are available to derive toxicological reference and drinking water guideline values for n-benzyl-alkylpyridium chloride. Additional discussion is included in the dossier provided in **Attachment 1**.

Based on its potential use as a biocide in produced water flow lines, n-benzyl-alkylpyridium chloride may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to n-benzyl-alkylpyridium chloride in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay), and treatment and retention (and associated biodecay) are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of the biocide in produced water would be diluted by a factor of at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system.

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an

---

<sup>3</sup> LD50 = lethal dose of 50 percent of population; mg/kg bw – milligrams per kilogram body weight



‘Unnamed tributary of the Dawson River’, not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

## Environmental Hazards

N-benzyl-alkylpyridium chloride exhibits significant acute and chronic aquatic toxicity. However, sediment dwelling organisms are far less sensitive to the substance perhaps based on combined effects of biodegradation and binding to the sediment matrix.

PNECs for n-benzyl-alkylpyridium chloride are provided in **Tables 3-5**. Experimental toxicity data on water organisms was available for two trophic levels to calculate PNECs in water. There are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method. PNEC calculations and assumptions are included in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson’s Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.



Further, estimated Water Management Facility (WMF) pond influent concentrations ( $7.2 \times 10^{-10}$  mg/L, refer **Attachment 2**) are well less than PNECs for aquatic receptors ( $5 \times 10^{-3}$  mg/L). Blending within the storage pond, degradation during storage and treatment would further reduce concentrations.

## References

AECOM. 2019. Revised Boron Site-Specific Water Quality Criterion – Dawson River Release Scheme. Letter from B. Goldsworthy and N. Lee to A. Lavery. 12 July 2019..

Australian Environmental Agency (AEA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia. Available: <https://www.nepc.gov.au/sites/default/files/2022-09/cmgt-nchem-eragm-industrial-chemicals-200902.pdf>

frc environmental. 2021. Santos GLNG Dawson River Watercourse Releases: Receiving Environment Monitoring Program. April 2021.



## Attachment 1 Risk Assessment Dossier



## N-benzyl-alkylpyridium chloride

This dossier on N-benzyl-alkylpyridium chloride presents the most critical studies pertinent to the risk assessment of this substance in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from The National Industrial Chemicals Notification and Assessment Scheme (NICNAS, 1994) and the ECHA database that provides information on chemicals that have been registered under the European Union (EU) REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – N-benzyl-alkylpyridium chloride was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. N-benzyl-alkylpyridium chloride was assessed as a tier 2 chemical for acute toxicity and chronic toxicity. Therefore, N-benzyl-alkylpyridium chloride is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

### 1 BACKGROUND

N-benzyl-alkylpyridium chloride is a mixture of alkyl pyridine quaternary ammonium salts. The substance is inherently biodegradable. Components show variable sorption to soils and sediments. It is not expected to bioaccumulate based on the experimental octanol water partition coefficient (log  $K_{ow}$ ). Very little information exists regarding the specific human health hazards associated with N-benzyl alkylpyridium chloride. Thus, the information provided in this dossier is taken from data collected for quaternary ammonium compounds in general. Significant absorption of quaternary ammonium compounds is unlikely due to their highly ionic nature. As the substance is corrosive (i.e., pH=1.2), very little toxicity data are available with the exception of acute toxicity data which indicates a low concern for human health hazards. In regard to environmental hazard, N-benzyl-alkylpyridium chloride exhibits significant acute and chronic aquatic toxicity. However, sediment dwelling organisms are far less sensitive to the substance based on combined effects of biodegradation and binding to the settlement matrix.

### 2 CHEMICAL NAME AND IDENTIFICATION

**Chemical Name (IUPAC):** 1-benzyl-1-methyl-2H-pyridin-1-ium; chloride

**CAS RN:** 68909-18-2

**Molecular formula:**  $C_{12}H_{17}ClNR_1R_2R_3R_4R_5$ , where R1-5 are alkyl groups

**Molecular weight:** 221.72 g/mol

**Synonyms:** Pyridinium, 1-(phenylmethyl)-, Et Me derivs., chlorides, Pyridinium, methyl-1-(phenylmethyl)-, chloride, N-Benzylpicolinonium chloride, Pyridinium, methyl-1-(phenylmethyl)-, chloride (1:1)

### 3 PHYSICAL AND CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

**Table 1 Overview of Physico-Chemical Properties of on N-benzyl-alkylpyridium chloride.**

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa*	Liquid	1	ECHA
Melting Point	-57.27 °C @ 101.3 kPa	1	ECHA
Boiling Point	116.34 °C @ 101.3 kPa	1	ECHA
Density	1,104 kg/m <sup>3</sup>	1	ECHA
Vapour Pressure	200 Pa @ 20°C	2	ECHA
Partition Coefficient (log K <sub>ow</sub> )	3 @ 25°C	2	ECHA
Water Solubility	100 g/L @ 30°C	1	ECHA
Viscosity	47.9 mm <sup>2</sup> /s (static) @ 38°C	-	ECHA

### 4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for N-benzyl-alkylpyridium chloride.

**Table 2 Existing International Controls**

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

### 5 ENVIRONMENTAL FATE SUMMARY

#### A. Summary

N-benzyl-alkylpyridium chloride is inherently biodegradable. Components show variable sorption to soils and sediments. It is not expected to bioaccumulate based on the experimental log K<sub>ow</sub>.

N-benzyl-alkylpyridium chloride exhibits significant acute and chronic aquatic toxicity. Sediment dwelling organisms are far less sensitive to the substance based on combined effects of biodegradation and binding to the settlement matrix.

## **B. Biodegradation**

The ready biodegradation of N-benzyl-alkylpyridium chloride in seawater was determined according to OCED guideline 306 (Biodegradability in Seawater). The rate of degradation was estimated at 13% in seawater assay. The substance was considered likely to be inherently biodegradable (ECHA) [KI Score=3].

## **C. Environmental Distribution**

A screening test conducted in accordance with OECD 121 indicated that due to its multi component nature, N-benzyl-alkylpyridium chloride displayed a range of Log  $K_{oc}$  values from <1.25 to 5.40. The substance is considered to be a UVCB substance comprising multiple components, of similar chemical functionality, in varying proportions. A quantitative assessment of these components would therefore present considerable technical difficulty as there is not considered to be an analytical method that is sufficiently sensitive, and so a more detailed assessment in accordance with OECD 106 for example would not be technically possible. For the purposes of this dossier, a log  $K_{oc}$  is estimated to be a midpoint of the range stated above (i.e., approximately 3).

## **D. Bioaccumulation**

No bioconcentration studies have been conducted on N-benzyl alkylpyridium chloride. N-benzyl alkylpyridium chloride is not expected to bioaccumulate based on the experimental log  $K_{ow}$  of 3 (ECHA) [KI. score = 1].

# **6 HUMAN HEALTH HAZARD ASSESSMENT**

## **A. Summary**

Very little information exists regarding the specific hazards associated with N-benzyl alkylpyridium chloride. Thus, the information provided in this section is taken from data collected for quaternary ammonium compounds in general.

Significant absorption of quaternary ammonium compounds is unlikely due to their highly ionic nature. As the substance is corrosive (i.e., pH=1.2), very little toxicity data are available with the exception of acute toxicity data showing a rat LD<sub>50</sub> of approximately 50 mg/kg-day.

## **B. Toxicokinetics**

No toxicokinetic data are available for these substances, however the data on related quaternary ammonium compounds are summarised below.

### Absorption

Significant absorption of quaternary ammonium compounds is unlikely due to their highly ionic nature. WHO (1998) reports the oral absorption of quaternary ammonium compounds in general to be poor. A published Canadian review of the toxicity of the quaternary ammonium compound didecyldimethylammonium chloride (DDAC) notes experiments in rats in which up to 99% of orally administered radioactivity was recovered in the faeces and less than 2.5% in the urine (ECHA 2020).

The dermal absorption of quaternary ammonium compounds is likely to be low based on the chemical structure, ionic nature, molecular weight and lack of lipophilicity of the substance. Absorption of this group of substances through skin is also indicated to be very low based on an absence of reports of systemic effects following dermal exposure (WHO, 1998). However, it is noted that the substance is corrosive, therefore it is possible that systemic absorption may occur following significant accidental dermal exposures resulting in skin burns, where the normal barrier integrity of the skin is compromised. Buist et al (2007) reported very low dermal penetration (0.5%) for the quaternary ammonium compound DDAC in human skin in vitro over a 48-hour period.

No data are available for absorption following inhalation exposure; however, it is considered unlikely that absorption by this route of exposure would be significant. Although not relevant to the human risk assessment, the WHO document notes that the systemic absorption of quaternary ammonium compounds following parenteral administration is 'possible'.

#### Distribution

No data on distribution are available. However, given the water solubility of the substance, it is likely to be widely distributed via the circulation if absorbed.

#### Metabolism

No data are available for the substance; however significant metabolism is not predicted given the likely poor systemic absorption. A published Canadian review of the toxicity of the quaternary ammonium compound DDAC reports some oxidative metabolism of the decyl sidechain, but no molecular cleavage by N-dealkylation (Henderson, 1992).

#### Excretion

Data indicate that quaternary ammonium compounds are largely excreted in the faeces (WHO, 1998; Henderson, 1992). The poor absorption and chemical nature of the substance (specifically the lack of lipophilicity) indicate that substance quaternary ammonium compounds have no or little potential for bioaccumulation.

### **C. Acute Toxicity**

The oral LD<sub>50</sub> in rats is 50.1 milligrams per kilogram (mg/kg, HPVIS) [Kl. score = 2]. There are no acute inhalation or dermal toxicity studies on N-benzyl-alkylpyridium chloride.

### **D. Irritation**

No studies are available. However, N-benzyl-alkylpyridium chloride is considered corrosive based on its pH of 1.2 (ECHA).

### **E. Sensitisation**

No studies are available.

### **F. Repeated Dose Toxicity**

No studies are available.

## G. Genotoxicity

The *in vitro* genotoxicity studies on N-benzyl-alkylpyridium chloride are presented in Table 3.

**Table 3 In vitro Genotoxicity Studies on N-benzyl-alkylpyridium chloride**

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation ( <i>S. typhimurium</i> strains)	-	-	1	ECHA
Mammalian cell gene mutation (mouse lymphoma L5178Y cells)	-	-	1	ECHA
Chromosomal aberrations (human lymphocytes)	-	-	1	ECHA

\*+, positive; -, negative

## H. Carcinogenicity

No studies are available.

## I. Reproductive Toxicity

No studies are available.

## J. Developmental Toxicity

No studies are available.

## K. Derivation of Toxicological Reference and Drinking Water Guidance Values

No data are available on N-benzyl-alkylpyridium chloride to derive oral toxicological reference and drinking water guidance values.

## L. Human Health Hazard Assessment Of Physico-Chemical Properties

N-benzyl-alkylpyridium chloride does not exhibit the following physico-chemical properties:

- Explosivity
- Oxidising potential

The substance is classified as flammable (Flam. Liquid 3).

## 7 ENVIRONMENTAL EFFECTS SUMMARY

### A. Summary

N-benzyl-alkylpyridium chloride exhibits significant acute and chronic aquatic toxicity. Sediment dwelling organisms are far less sensitive to the substance perhaps based on combined effects of biodegradation and binding to the sediment matrix.

## B. Aquatic Toxicity

Table 4 lists the results of acute aquatic toxicity studies on salts of N-benzyl-alkylpyridium chloride.

**Table 4 Acute Aquatic Toxicity Studies on N-benzylalkylpyridium chloride**

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
<i>Cyprinodon variegatus</i>	96-hr LC <sub>50</sub>	14.1	1	ECHA
<i>Daphnia magna</i>	48-hr EC <sub>50</sub>	3.1	1	ECHA
<i>Pseudokirchneriella subcapitata</i>	72-hr EC <sub>50</sub>	0.47	1	ECHA

## C. Terrestrial Toxicity

No studies are available.

## D. Calculation of PNEC

The PNEC calculations for N-benzyl-alkylpyridium chloride follow the methodology discussed in DEWHA (2009).

### PNEC water

Experimental results are available for two trophic levels. Acute EC<sub>50</sub> values are available for *Daphnia* (3.1 milligrams per litre [mg/L]), and algae (0.47 mg/L). On the basis that the data consists of short-term results from two trophic levels, an assessment factor of 1,000 has been applied to the lowest reported E(L)C<sub>50</sub> value of 0.47 mg/L for algae. The PNEC<sub>water</sub> is 0.00047 mg/L.

### PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Therefore, the PNEC<sub>sed</sub> was calculated using the equilibrium partitioning method. The PNEC<sub>sed</sub> is 0.0073 mg/kg wet weight.

The calculations are as follows:

$$\begin{aligned}
 \text{PNEC}_{\text{sed}} &= (K_{\text{sed-water}}/\text{BD}_{\text{sed}}) \times 1000 \times \text{PNEC}_{\text{water}} \\
 &= (20/1280) \times 1000 \times 0.00047 \\
 &= 0.0073 \text{ mg/kg}
 \end{aligned}$$

Where:

$K_{\text{sed-water}}$  = suspended matter-water partition coefficient (m<sup>3</sup>/m<sup>3</sup>)

$\text{BD}_{\text{sed}}$  = bulk density of sediment (kg/m<sup>3</sup>) = 1,280 [default]

$\text{PNEC}_{\text{water}}$  = 0.00047 mg/L

$$\begin{aligned}
 K_{\text{sed-water}} &= 0.8 + [0.2 \times K_{\text{p}_{\text{sed}}}/1000 \times \text{BD}_{\text{solid}}] \\
 &= 0.8 + [(0.2 \times 40)/1000 \times 2400] \\
 &= 20 \text{ m}^3/\text{m}^3
 \end{aligned}$$

$K_{p_{sed}}$  = solid-water partition coefficient (L/kg)

$BD_{solid}$  = bulk density of the solid phase ( $kg/m^3$ ) = 2,400 [default]

And:

$$K_{p_{sed}} = K_{oc} \times f_{oc}$$

$$= 1000 \times 0.04$$

$$= 40 \text{ L/kg}$$

Where:

$K_{oc}$  = organic carbon normalised distribution coefficient (L/kg). The  $K_{oc}$  for sediment is 1000.

$f_{oc}$  = fraction of organic carbon suspended sediment = 0.04 [default].

### PNEC soil

There are no  $EC_{10}$  or NOEC values for terrestrial receptors. Therefore, the  $PNEC_{soil}$  was calculated using the equilibrium partitioning method. The  $PNEC_{soil}$  is 0.0063 mg/kg soil dry weight.

The calculations are as follows:

$$PNEC_{soil} = (K_{p_{soil}}/BD_{soil}) \times 1000 \times PNEC_{water}$$

$$= (20/1500) \times 1000 \times 0.00047$$

$$= 0.0063 \text{ mg/kg soil dry weight}$$

Where:

$K_{p_{soil}}$  = soil-water partition coefficient ( $m^3/m^3$ )

$BD_{soil}$  = bulk density of soil ( $kg/m^3$ ) = 1,500 [default]

$PNEC_{water}$  = 0.00047 mg/L

$$K_{p_{soil}} = K_{oc} \times f_{oc}$$

$$= 1000 \times 0.02$$

$$= 20 \text{ m}^3/\text{m}^3$$

Where:

$K_{oc}$  = organic carbon normalised distribution coefficient (L/kg). The  $K_{oc}$  was estimated to be 1000 L/kg.

$f_{oc}$  = fraction of organic carbon in soil = 0.02 [default].

## **8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN**

### **A. PBT Categorisation**

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (ICHEMS, 2022; ECHA, 2017).

N-benzyl alkylpyridium chloride is estimated to be ultimately biodegradable.

No bioconcentration studies are available for N-benzyl alkylpyridium chloride. However, the measured log  $K_{ow}$  for N-benzyl alkylpyridium chloride is 3; thus, N-benzyl alkylpyridium chloride does not meet the screening criteria for bioaccumulation.

The acute  $EC_{50}$  values for N-benzyl alkylpyridium chloride in algae is <1 mg/L. Thus, N-benzyl alkylpyridium chloride meets the screening criteria for toxicity.

The overall conclusion is that N-benzyl alkylpyridium chloride is not a PBT substance.

**B. Other Characteristics of Concern**

No other characteristics of concern were identified for N-benzyl-alkylpyridium.



9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment <sup>1</sup>	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required <sup>3</sup>
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity <sup>2</sup>	Chronic Toxicity <sup>2</sup>	
N-benzyl-alkylpyridium chloride	68909-18-2	Not a PBT	No	No	No	No	No	Yes	2	No Data	2

Footnotes:

- 1 - PBT Assessment based on PBT Framework.  
2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).  
3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

PBT = Persistent, Bioaccumulative and Toxic  
B = bioaccumulative  
P = persistent  
T = toxic

## 10 REFERENCES, ABBREVIATIONS AND ACRONYMS

### A. References

- Buist, Harrie E, Cees de Heer, Johan A van Burgsteden, Johannes J M van de Sandt. (2007). Dermatokinetics of didecyldimethylammonium chloride and the influence of some commercial biocidal formulations on its dermal absorption in vitro. *Regul Toxicol Pharmacol*. 2007 Jun; 48(1):87-92.
- Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia. Available: <https://www.nepc.gov.au/sites/default/files/2022-09/cmgt-nchem-eragm-industrial-chemicals-200902.pdf>
- Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra. Available: [www.environment.gov.au/water/coal-and-coal-seam-gas/national-assessment-chemicals/consultation-risk-assessment-guidance-manual](http://www.environment.gov.au/water/coal-and-coal-seam-gas/national-assessment-chemicals/consultation-risk-assessment-guidance-manual)
- ECHA. ECHA REACH database: <http://echa.europa.eu/information-on-chemicals/registered-substances>.
- European Chemicals Agency [ECHA]. (2017). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland. Henderson. Available: <https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment>
- ECHA 2020. Registration dossier for Quaternary ammonium compounds, di-C12-18-alkyldimethyl, chlorides. <https://echa.europa.eu/bg/registration-dossier/-/registered-dossier/11882/7/2/2>
- HPVIS. The U.S. EPA High Production Volume Information System: [https://iaspub.epa.gov/opphpv/public\\_search.html\\_page](https://iaspub.epa.gov/opphpv/public_search.html_page)
- Industrial Chemicals Environmental Management Standard [IChEMS]. (2022). Australian Environmental Criteria for Persistent, Bioaccumulative and/or Toxic Chemicals. Available: <https://www.dcceew.gov.au/sites/default/files/documents/australian-pbt-criteria.pdf>
- Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. *Regul. Toxicol. Pharmacol*. 25:1-5.
- NICNAS (1994). National Industrial Chemicals Notification and Assessment Scheme (NICNAS), AGPS, Canberra, Australia.

WHO. (1998). International Programme on Chemical Safety (IPCS). Quaternary ammonium (PIM G022). <http://www.inchem.org/documents/pims/chemical/pimg022.htm>

## B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
COC	constituent of concern
DDAC	didecyldimethylammonium chloride
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm <sup>3</sup>	grams per cubic centimetre
g/L	grams per litre
IChEMS	Industrial Chemicals Environmental Management Standard
IUPAC	International Union of Pure and Applied Chemistry
kg/m <sup>3</sup>	kilograms per cubic metre
KI	Klimisch scoring system
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LD	lethal dose
m <sup>3</sup>	cubic metre
mg/kg	milligrams per kilogram
mg/kg-day	milligrams per kilogram per day
mg/L	milligrams per litre
mm <sup>2</sup> /s	square millimetre per second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOEC	no observed effects concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal

PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials
WHO	World Health Organization



## Attachment 2 Contingency Biocide Dosing Assumptions

**Attachment 2**  
**Summary of Exposure Point Concentration Development**  
**(Contingency Water Treatment Chemicals)**

## Mass Balance

In other Santos project areas, approximately 413 milligrams per litre (mg/L) of a water treatment product is being dosed (9.2 litres [L] added to approximately 1,380 billion barrels [bbl] or  $2.2 \times 10^5$  litres of legacy/CF1 PFW). The constituent of potential concern (COPC) legacy/CF1 produced formation water (PFW) concentrations are calculated based on the product dose that is apportioned between the COPCs based on the COPC percent weight in the product (composition information in the safety data sheet). The concentration of the COPCs in the water storage pond influent (representative of treatment of combined produced water from legacy/CF1 PFW and bore water) was based on the combined dilution from 2,300 bbl/day.

On this basis, the concentration of COPCs in the water storage pond influent are calculated as follows:

COPC	CAS Number	Percent Weight Product	COPC Legacy/CF1 PFW (mg/L)	Storage Pond Influent (mg/L)
Benzyl-C1-2-alkylpyridinium chloride	68909-18-2	5	1.0E-04	7.2E-10

CAS = Chemical Abstracts Service

COPC = constituent of potential concern

mg/L = milligrams per litre

PFW = produced formation water