Quaternary Ammonium Compounds, Benzyl(hydrogenated tallow alkyl)dimethyl, Salts with Bentonite (CAS# 71011-24-0) GreenScreen® for Safer Chemicals (GreenScreen®) Assessment

Prepared for:

Washington State Department of Ecology

Prepared by:

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Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite are a chemical that is used in coatings and paints, drilling muds, printing inks, cosmetics, and nanocomposites.

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite was assigned a GreenScreen® Benchmark Score of 2 ("Use but Search for Safer Substitutes") as it has Very High persistence (P) and Moderate Ecotoxicity (chronic aquatic toxicity (CA)). This corresponds to GreenScreen® benchmark classification 2c in CPA 2011. Data gaps (DG) exist for endocrine activity (E), neurotoxicity, single dose and repeated dose (Ns and Nr*), and respiratory sensitization (SnR*). As outlined in CPA (2013) Section 12.2 (Step 8 – Conduct a Data Gap Analysis to assign a final Benchmark score), quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite meets the requirements for a GreenScreen® Benchmark Score of 2 chemical despite the data gaps. In a worst-case scenario, if quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite were assigned a High score for the data gaps endocrine activity (E), neurotoxicity repeated dose (Nr*) or respiratory sensitization (SnR*), it would be categorized as a Benchmark 1 Chemical.

GreenScreen® Benchmark Score for Relevant Route of Exposure:
As a standard approach for GreenScreen® evaluations, all exposure routes (oral, dermal, and inhalation) were evaluated together, so the GreenScreen® Benchmark Score of 2 ("Use but Search for Safer Substitutes") is applicable for all routes of exposure.

GreenScreen® Hazard Ratings for Quaternary Ammonium Compounds, Benzyl(hydrogenated tallow alkyl)dimethyl, Salts with Bentonite

Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
						single	repeated*	single	repeated*										
L	**L**	**L**	**L**	DG	**L**	**L**	**L**	DG	DG	**L**	DG	**L**	*M*	**L**	**M**	*vH*	*L*	**L**	**L**

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect estimated values, authoritative B lists, screening lists, weak analogues, and lower confidence. Hazard levels in **BOLD** font are used with good quality data, authoritative A lists, or strong analogues. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e., vH, H, M, and L) instead of three (i.e., H, M, and L), and are based on single exposures instead of repeated exposures. Please see Appendix A for a glossary of hazard acronyms.

GreenScreen® Assessment for Quaternary Ammonium Compounds, Benzyl(hydrogenated tallow alkyl)dimethyl, Salts with Bentonite (CAS #71011-24-0)

Method Version: GreenScreen® Version 1.2[1]
Assessment Type[2]: Certified

Chemical Name: Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite

CAS Number: 71011-24-0

GreenScreen® Assessment Prepared By:
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Organization: ToxServices LLC
Date: October 14, 2014
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Name: Bingxuan Wang, Ph.D.
Title: Toxicologist
Organization: ToxServices LLC
Date: October 16, 2014

Confirm application of the *de minimus* rule[3]: N/A

Chemical Structure(s):
The quaternary ammonium compounds (cations) have the following general formula:

$N^+R_1R_2R_3R_4$

Where R_n are substitutions on the nitrogen atom:

Methyl – 2 substitutions
Alkyl (C14-22) – 2 substitutions

The clays (anions) are made of silicon, hydrogen, oxygen, sodium, calcium, aluminum, and magnesium (bentonite) (OECD 2007).

Also called: Dimethyl benzyl hydrogenated tallow ammonium chloride reaction product with bentonite; Hydrogenated tallow alkyl dimethyl benzyl ammonium bentonite salts
Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compds. with bentonite (ChemIDplus 2014)

Chemical Structure(s) of Chemical Surrogates Used in the GreenScreen®:
A limited dataset was available for quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite. Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite is a member of OECD's category of Organoclays. Organoclay compounds are smectite clays reacted with quaternary ammonium compounds. All smectite clays are structurally similar, negatively charged two-dimensional inorganic polymers with a layered structure, and form organoclay compounds when the sodium and calcium cations associated with the clay are exchanged for quaternary ammonium compounds that become held tightly to the clay. Due to similarity

[1] Use GreenScreen® Assessment Procedure (Guidance) V1.2

[2] GreenScreen® reports are either "UNACCREDITED" (by unaccredited person), "AUTHORIZED" (by Authorized GreenScreen® Practitioner), "CERTIFIED" (by Licensed GreenScreen® Profiler or equivalent) or "CERTIFIED WITH VERIFICATION" (Certified or Authorized assessment that has passed GreenScreen® Verification Program)

[3] Every chemical in a material or formulation should be assessed if it is:
1. intentionally added and/or
2. present at greater than or equal to 100 ppm

in structure and chemical characteristics, OECD evaluated Organoclays as a class, using a read across approach to apply available data for members of the class to fill data gaps for other members. Data for the following members of the Organoclays category were used to fill data gaps for quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite:

- Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with bentonite (CAS# 68953-58-2)
- Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with hectorite (CAS# 71011-26-2)
- Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with hectorite (CAS# 71011-27-3)
- Quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, salts with hectorite (CAS# 121888-67-3)
- Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 68953-58-2)

Chemical structures for the aforementioned structures are unspecified. Despite the use of surrogates, data gaps remain for endocrine activity, neurotoxicity (single dose and repeated dose), and respiratory sensitization.

Due to the significant degree of structural similarity and physicochemical properties between these chemicals and quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite, the surrogates identified above are considered to be strong surrogates for quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite by ToxServices.

Identify Applications/Functional Uses: (OECD 2007)
1. Coatings and paints
2. Drilling muds
3. Printing inks
4. Cosmetics
5. Nanocomposites

GreenScreen® Summary Rating for Quaternary Ammonium Compounds, Benzyl(hydrogenated Tallow alkyl)dimethyl, Salts with Bentonite[4]: Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite was assigned a GreenScreen® Benchmark Score of 2 ("Use but Search for Safer Substitutes") as it has Very High persistence (P) and Moderate Ecotoxicity (chronic aquatic toxicity (CA)). This corresponds to GreenScreen® benchmark classification 2c in CPA 2011. Data gaps (DG) exist for endocrine activity (E), neurotoxicity, single dose and repeated dose (Ns and Nr*), and respiratory sensitization (SnR*). As outlined in CPA (2013) Section 12.2 (Step 8 – Conduct a Data Gap Analysis to assign a final Benchmark score), quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite meets the requirements for a GreenScreen® Benchmark Score of 2 chemical despite the data gaps. In a worst-case scenario, if quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite were assigned a High score for the data gaps endocrine activity (E), neurotoxicity repeated dose (Nr*) or respiratory sensitization (SnR*), it would be categorized as a Benchmark 1 Chemical.

[4] For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation potential, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.

Figure 1: GreenScreen® Hazard Ratings for Quaternary Ammonium Compounds, Benzyl(hydrogenated tallow alkyl)dimethyl, Salts with Bentonite

Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
						single	repeated*	single	repeated*										
L	L	L	L	DG	L	L	L	DG	DG	L	DG	L	*M*	L	M	*vH*	*L*	L	L

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect estimated (modeled) values, authoritative B lists, screening lists, weak analogues and lower confidence. Hazard levels in **BOLD** font are used with good quality data, authoritative A lists, or strong analogues. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e. vH, H, M, and L) instead of three (i.e. H, M, and L), and are based on single exposures instead of repeated exposures. Please see Appendix A for a glossary of hazard acronyms.

Transformation Products and Ratings:

Identify feasible and relevant fate and transformation products (i.e., dissociation products, transformation products, valence states) **and/or moieties of concern**[5]

The organic portion of quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite undergoes combustion at 180°C, producing carbon dioxide, water, and nitrogen oxides, which are naturally occurring in the environment. After combustion, naturally occurring bentonite clay (CAS# 1302-78-9) remains. Organoclay compounds do not undergo hydrolysis (OECD 2007), and dissociation of the quaternary ammonium compounds bound to the clay surface requires strong ionic and adsorption forces to be overcome simultaneously, which is unlikely to occur outside of a laboratory.

Functional Use	Life Cycle Stage	Transformation Pathway	Transformation Products	CAS #	Feasible and Relevant?	List Translator Results[6,7]
Not identified	Not identified	Combustion	Bentonite	1302-78-9	Yes	LT-U

Introduction

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite are a reaction product of bentonite clay with quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides. Bentonite clay carries a negative charge that attracts naturally occurring sodium and calcium ions to the surface, and organoclay compounds such as quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, and chlorides are produced when these cations are exchanged for quaternary ammonium cations. The result is a highly hydrophobic organoclay compound with tightly bound quaternary ammonium cations. Quaternary ammonium compounds,

[5] A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.
[6] The GreenScreen® List Translator identifies specific authoritative or screening lists that should be searched to screen for GreenScreen® benchmark 1 chemicals (CPA 2012b). Pharos (Pharos 2014) is an online list-searching tool that is used to screen chemicals against the lists in the List Translator electronically.
[7] The way you conduct assessments for transformation products depends on the Benchmark Score of the parent chemical (See Guidance).

benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite are used in coatings and paints, drilling muds, printing inks, cosmetics, and nanocomposites (OECD 2007).

ToxServices assessed quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite against GreenScreen® Version 1.2 (CPA 2013) following procedures outlined in ToxServices' SOP 1.69 (GreenScreen® Hazard Assessment) (ToxServices 2013).

GreenScreen® List Translator Screening Results

The GreenScreen® List Translator identifies specific authoritative or screening lists that should be searched to identify GreenScreen® benchmark 1 chemicals (CPA 2012b). Pharos (Pharos 2014) is an online list-searching tool that is used to screen chemicals against the List Translator electronically. It checks all of the lists in the List Translator with the exception of the U.S. Department of Transportation (U.S. DOT) lists (U.S. DOT 2008a,b) and these should be checked separately in conjunction with running the Pharos query. The output indicates benchmark or possible benchmark scores for each human health and environmental endpoint. The output for quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite can be found in Appendix C and a summary of the results can be found below:

- PBT
  - DSL: DSL Substances that are Bioaccumulative
- Restricted List
  - DSL: Inherently Toxic in the Environment

PhysicoChemical Properties of Quaternary Ammonium Compounds, Benzyl(hydrogenated tallow alkyl)dimethyl, Salts with Bentonite

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite are a solid at room temperature and the organic moiety decomposes at elevated temperatures. This substance is not soluble and does not dissociate in water, neither is it soluble in organic solvents, making it impossible to measure or model the partition coefficient.

Table 1: Physical and Chemical Properties of Quaternary Ammonium Compounds, Benzyl(Hydrogenated tallow alkyl)dimethyl, Salts with Bentonite (CAS #71011-24-0)

Property	Value	Reference
Molecular formula	Unspecified	ChemIDplus 2014
SMILES Notation	Unspecified	ChemIDplus 2014
Molecular weight	Unspecified	ChemIDplus 2014
Physical state	Solid	OECD 2008a
Appearance	Powder	OECD 2008a
Melting point	Decomposes at 180ºC (organic portion)	OECD 2008a
Vapor pressure	Negligible up to 200ºC	OECD 2008a
Water solubility	Insoluble	OECD 2007
Dissociation constant	Not applicable	
Density/specific gravity	Not identified	OECD 2008a
Partition coefficient	Not feasible/applicable	OECD 2008a

Hazard Classification Summary Section:

Group I Human Health Effects (Group I Human)

Carcinogenicity (C) Score (H, M, or L): *L*
Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite were assigned a score of Low for carcinogenicity based on the lack of evidence for respiration, absorption, or carcinogenicity for this chemical. GreenScreen® criteria classify chemicals as a Low hazard for carcinogenicity when adequate data are available and are negative for carcinogenicity, no structural alerts are available, and the chemical is not classified for this endpoint under GHS or on authoritative lists (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists
- No data were identified.
- OECD 2007
  - Based on the particle size and distribution information provided by the suppliers of these organoclays, these materials are not expected to be respirable or absorbed through the skin.
- Based on the insolubility of organoclays in water and lipids, the lack of evidence of tissue retention and uptake after oral ingestion, and the lack of skin absorption, the carcinogenic potential of organoclays via oral and dermal routes of exposure is expected to be low. Inhalation of insoluble particles may be a carcinogenicity concern, such as titanium dioxide and carbon black, which are listed as carcinogens by authoritative bodies. However, as the reported particle sizes and distribution indicate that they are not respirable, the carcinogenic potential through inhalation is also expected to be low. This evaluation is also supported by the overall low toxicity profile of this substance below. Due to lack of measured data for this endpoint, the score is italicized.

Mutagenicity/Genotoxicity (M) Score (H, M, or L): L
Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite was assigned a score of Low for mutagenicity/genotoxicity based on *in vitro* mutagenicity data for quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite and other organoclays, and *in vitro* and *in vivo* clastogenicity for other organoclays. GreenScreen® criteria classify chemicals as a Low hazard for mutagenicity/genotoxicity when adequate data are available and are negative for mutagenicity and clastogenicity, and the chemical is not present on authoritative or screening lists (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with bentonite (CAS# 71011-24-0)

- OECD 2008a
  - Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with bentonite was negative in a bacterial reverse mutation assay in *S .typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98, and TA 100 at doses of 50, 150, 500, 1,500, and 5,000 µg/plate with and without metabolic activation.
  - Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with bentonite was negative in an *in vivo* micronucleus assay in rat (5/sex) bone marrow 24 hours after oral administration of 1 or 1,000 mg/kg/day for 28 days. There was

no significant increase in the frequency of micronucleated polychromatic erythrocytes and no significant decrease in the ratio of polychromatic to normochromatic erythrocytes.

- Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with bentonite was negative for chromosomal aberrations in an *in vivo* cytogenetics assay in rat (5/sex) lymphocytes in rats administered 1 or 1,000 mg/kg/day for 28 days. Cells were evaluated after 48 hours of culture post-harvest, and no increase in chromosomal damage was seen.

Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 68953-58-2)

- OECD 2008b
  - Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite was negative in a GLP compliant Ames reverse mutation assay in *S. typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98, and TA 100 at doses of 10, 30, 100, 300, 1,000 and 3,000 µg/plate with and without metabolic activation.

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with hectorite (CAS# 71011-26-2)

- OECD 2007
  - Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with hectorite was negative in a bacterial reverse mutation assay in *S .typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98, and TA 100 at doses of 50, 150, 500, 1,500, and 5,000 µg/plate with and without metabolic activation.
  - Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with hectorite was negative in an in vitro mammalian cell mutagenicity assay in mouse lymphoma cells (TK +/- locus of L5178Y) at concentrations of 1 to 50 µg/mL without metabolic activation and 5 to 70 µg/mL with metabolic activation.

Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with hectorite (CAS# 71011-27-3)

- OECD 2007
  - Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with hectorite was negative in a bacterial reverse mutation assay in *S. typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98, and TA 100 at doses of 17, 50, 167, 500, 1,667, and 5,000 µg/plate with and without metabolic activation.

Quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, salts with hectorite (CAS# 121888-67-3)

- OECD 2007
  - Quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, salts with hectorite was negative in an *in vivo* micronucleus assay in rat (5/sex) bone marrow 24 hours after oral administration of 1 or 1,000 mg/kg/day for 28 days. There was no significant increase in the frequency of micronucleated polychromatic erythrocytes and no significant decrease in the ratio of polychromatic to normochromatic erythrocytes.
  - Quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, salts with hectorite was negative for chromosomal aberrations in an *in vivo* cytogenetics assay in rat (5/sex) lymphocytes in rats administered 1 or 1,000 mg/kg/day for 28 days. Cells were evaluated after 48 hours of culture post-harvest, and no increase in chromosomal damage was seen.

Reproductive Toxicity (R) Score (H, M, or L): L

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite was assigned a score of Low for reproductive toxicity based on a 1-generation reproductive and developmental toxicity study for another organoclay compound. GreenScreen® criteria classify chemicals as a Low hazard for reproductive toxicity when adequate data are available and are negative for reproductive toxicity, and the chemical is not present on authoritative or screening lists (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* Not present on any screening lists

<u>Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 71011-24-0)</u>

- No data were identified for this endpoint.

<u>Quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, salts with hectorite (CAS# 121888-67-3)</u>

- OECD 2007, 2008c
    - Quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, salts with hectorite were tested in a GLP-compliant 1-generation reproduction and developmental toxicity study according to OECD Guideline 415 in Sprague-Dawley rats. Animals (24/sex/dose) were administered 0, 50, 225, or 1,000 mg/kg/day via gavage once daily for 74 days prior to mating and during mating (males) or 18 days prior to mating through lactation day 21 (females). Offspring were sacrificed on lactation day 21. No effects on mating and pregnancy indices, pre-coital interval, gestation length, or gestation and parturition index were seen. OECD identified a NOAEL of 1,000 mg/kg/day for reproductive toxicity based on the lack of effects.

Developmental Toxicity incl. Developmental Neurotoxicity (D) Score (H, M, or L): L

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite was assigned a score of Low for developmental toxicity based on a 1-generation reproductive and developmental toxicity study for another organoclay compound. GreenScreen® criteria classify chemicals as a Low hazard for developmental toxicity when adequate data are available and are negative for developmental toxicity, and the chemical is not present on authoritative or screening lists (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* Not present on any screening lists

<u>Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 71011-24-0)</u>

- No data were identified for this endpoint.

<u>Quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, salts with hectorite (CAS# 121888-67-3)</u>

- OECD 2007, 2008c
    - In the GLP-compliant 1-generation reproduction and developmental toxicity study according to OECD Guideline 415 in Sprague-Dawley rats described above for reproductive toxicity, animals (24/sex/dose) were administered 0, 50, 225, or 1,000 mg/kg/day via gavage once daily for 74 days prior to mating and during mating (males) or 18 days prior to mating through lactation day 21 (females). Offspring were sacrificed on lactation day 21. No effects birth index and viability indices; sex ratio, offspring physical development, clinical

signs, or reflexes were seen. Mean litter weight from day 7-21 of lactation was reduced but was not considered to be toxicologically significant. OECD identified a NOAEL of 1,000 mg/kg/day for developmental toxicity based on the lack of effects.

Endocrine Activity (E) Score (H, M, or L): DG
Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite were assigned a score of data gap for endocrine disruption based on a lack of data for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists
- Not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- Not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.
- No data were identified for this endpoint.

Group II and II* Human Health Effects (Group II and II* Human)
Note: Group II and Group II* endpoints are distinguished in the v 1.2 Benchmark system. For Systemic Toxicity and Neurotoxicity, Group II and II* are considered sub-endpoints and test data for single or repeated exposures may be used. If data exist for single OR repeated exposures, then the endpoint is not considered a data gap. If data are available for both single and repeated exposures, then the more conservative value is used.

Acute Mammalian Toxicity (AT) Group II Score (vH, H, M, or L): L
Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite was assigned a score of Low for acute toxicity based on acute oral and inhalation LD/LC_{50} values in rats. GreenScreen® criteria classify chemicals as a Low hazard for acute toxicity when oral LD_{50} values are greater than 2,000 mg/kg and inhalation LC_{50} values are greater than 5 mg/L (dust), and the chemical is not present on authoritative or screening lists (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 71011-24-0)

- OECD 2008a
  - *Inhalation:* LC_{50} (rat, male and female Sprague-Dawley) = greater than 5.2 mg/L/4h

Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 68953-58-2)

- OECD 2008b
  - *Oral*: LD_{50} (rat, male and female albino) = greater than 5,000 mg/kg
  - *Oral*: LD_{50} (rat, male and female Wistar) = greater than 5,000 mg/kg
  - *Oral*: LD_{50} (rat, male and female, strain not specified) = greater than 8,000 mg/kg
  - *Oral*: LD_{50} (rat, male and female Wistar) = greater than 5,000 mg/kg
  - *Inhalation*: LC_{50} (rat, male and female Sprague-Dawley) = greater than 12.7 mg/L/4h
  - *Inhalation*: LC_{50} (rat, male and female Sprague-Dawley) = greater than 5.7 mg/L/4h
  - *Inhalation*: LC_{50} (rat, male and female albino) = greater than 200 mg/L/1h

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST)
Group II Score (single dose) **(vH, H, M, or L): L**
Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite was assigned a score of Low for systemic toxicity (single dose) based on acute oral and inhalation toxicity studies in rats. GreenScreen® criteria classify chemicals as a Low hazard for systemic toxicity (single dose) when no adverse systemic effects are seen below the guidance values of 2,000 mg/kg for an acute oral toxicity study or 5.0 mg/L for an acute inhalation toxicity (dust) study (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* Not present on any screening lists

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 71011-24-0)

- OECD 2008a
    - *Inhalation:* In the acute inhalation toxicity study in male and female Sprague-Dawley rats that identified an LC_{50} of > 5.2 mg/L/4h, no mortality was observed. Treatment caused nasal discharge in 7 animals on day 2. One treated animal had difficulty breathing on days 2 and 3. Treatment produced a transient decrease in weight gain in male and female rats on day 4 that was reversed by day 8. Necropsy found no treatment-related lesions or abnormalities.

Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 68953-58-2)

- OECD 2008a
    - *Oral*: In the acute oral toxicity study in male and female albino rats that identified an LD_{50} greater than 5,000 mg/kg, no signs of toxicity were observed.
    - *Oral*: In the acute oral toxicity study in male and female Wistar rats that identified an LD_{50} greater than 5,000 mg/kg, no mortality or effects on body weight were observed.
    - *Oral*: In the acute oral toxicity study in male and female Wistar rats that identified an LD_{50} greater than 5,000 mg/kg, no mortality, effects on clinical signs, or treatment-related effects on body weight were seen.
    - *Inhalation*: In the acute inhalation toxicity study in male and female Sprague-Dawley rats that identified an LC_{50} greater than 12.7 mg/L/4h, no mortality was observed, and there were no treatment-related effects on body weight or necropsy observed.
    - *Inhalation*: In the acute inhalation toxicity study in male and female Sprague-Dawley rats that identified an LC_{50} greater than 5.7 mg/L/4h, no mortality was observed, and there were no treatment-related clinical signs, effects on body weight, or gross necropsy observed.
- Based on the results summarized above, no signs of significant toxicity or organ effects were noted in single exposure toxicity studies of quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite and quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite.

Group II* Score (repeated dose) **(H, M, or L): L**
Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite were assigned a score of Low for systemic toxicity (repeated dose) based on a subchronic oral toxicity study in rats. GreenScreen® criteria classify chemicals as a Low hazard for systemic toxicity (repeated dose) when adequate data are available and no adverse effects are seen below the guidance value of 100 mg/kg/day for an oral study (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists

- *Screening:* Not present on any screening lists

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with bentonite (CAS# 71011-24-0)

- OECD 2008c
  - *Oral*: In a subchronic oral toxicity study in male and female Charles River rats, animals (5/sex/dose) were administered 0 or 1,000 mg/kg/day via gavage for 28 days. No mortality, clinical signs of toxicity, or effects on body weight, food consumption, hematology, or clinical chemistry, were observed. Relative liver weights were significantly decreased in females, but this effect was not considered to be toxicologically relevant due to the absence of macroscopic or microscopic findings. OECD identified a NOAEL of 1,000 mg/kg/day.

Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 68953-58-2)

- OECD 2008b
  - *Oral*: Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite were tested in a subchronic dietary study in male and female rats (strain not specified). Animals (6/sex/dose) were administered diets containing 0, 1, 5, or 25% (approximately 500 to 1,000, 2,500 to 5,000, or 12,500 to 25,000 mg/kg/day, respectively) quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite for 12 weeks. Food consumption, body weight, and clinical signs were recorded. Hematological examinations were performed on 2 rats/group. Liver and kidney weights were recorded at necropsy and sections of large intestine of 2 rats/sex/group were submitted for histopathology. No treatment related mortality occurred. Growth rate was not affected at the low and mid dose, but was reduced at the high dose due to the lower caloric value of the diet. No hematological changes, gross abnormalities, or effects on liver and kidney weight were seen. Histopathology revealed irritation of the large intestine, which was seen in all dose groups including controls and was not considered to be treatment related. Clinical chemistry was not evaluated. OECD identified a NOAEL of 25% in the diet (12,500 to 25,000 mg/kg/day).
  - *Dermal*: In a subchronic dermal toxicity study in albino rabbits (sex and strain not specified), animals (10/dose) were dermally administered 0.5 g moistened Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite to the back for 6 hours/day, 5 days/week, for 90 days. Blood hemoglobin levels and complete blood counts were recorded, and liver, kidney, and skin were submitted for histopathology. Livers of treated animals showed increased glycogen storage and no parenchymal damage. Nearly all livers in treated and control animals showed evidence of parasitic infection. Signs of acute glomerulitis and tubular damage in the kidney were potentially due to parasitic infection. No signs of local of systemic toxicity were apparent. There were no significant effects on blood hemoglobin levels, white or red blood cell counts, or gross pathology. OECD considered this study to be invalid due to the use of a single dose level and an insufficient number of animals.

Quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, salts with hectorite (CAS# 121888-67-3)

- OECD 2008c
  - *Oral*: In a subchronic oral toxicity study in male and female Charles River rats, animals (5/sex/dose) were administered 0 or 1,000 mg/kg/day via gavage for 28 days. No mortality, clinical signs of toxicity, effects on body weight or food consumption, hematological changes, or abnormalities in gross or microscopic pathology were observed. Mean thrombotest time and chloride and calcium levels were significantly reduced in treated

females. Adrenal weights were significantly increased in males but this effect was not considered toxicologically significant in the absence of pathological changes. OECD identified a LOAEL of 1,000 mg/kg/day, the only dose studied, based on changes in thrombotest time and calcium and chloride levels in females.

Neurotoxicity (N)
***Group II Score (single dose)* (vH, H, M, or L):** DG
Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite were assigned a score of Data Gap for neurotoxicity (single dose) based on a lack of data for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006, 2014).
- No data were identified for this endpoint.

***Group II* Score (repeated dose)* (H, M, or L):** DG
Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite were assigned a score of Data Gap for neurotoxicity (repeated dose) based on a lack of data for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006, 2014).
- No data were identified for this endpoint.

Skin Sensitization (SnS) Group II* Score (H, M, or L): L
Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite were assigned a score of Low for skin sensitization based on negative findings in a guinea pig maximization test. GreenScreen® criteria classify chemicals as a Low hazard for skin sensitization when adequate data are available and are negative for sensitization, and the chemical is not present on authoritative or screening lists (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists

<u>Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 68953-58-2)</u>

- OECD 2008a
  - Quaternary ammonium compounds, benzyl(hyddrogenzted tallow alkyl)dimethyl, salts with bentonite was not sensitizing in a guinea pig maximization test in guinea pigs (sex and strain not specified). Animals were induced with a series of intracutaneous injections of a 5% suspension and challenged with a topical application of 30% and 15% suspension. No evidence of skin reaction was seen at challenge.

<u>Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 68953-58-2)</u>

- OECD 2008b
  - Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite was not sensitizing in an intracutaneous test in guinea pigs (sex and strain not

specified). A 0.1% suspension was administered intracutaneously three times/week for a total of 10 doses (0.05 mL for the first dose and 0.1 mL for subsequent doses). Animals were challenged after 2 weeks with 0.05 mL of the suspension by injection and ratings were made according to the scoring system of Draize. No evidence of a skin reaction was seen at challenge.

- Products containing 4.1 or 4.0% quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite were negative in a human repeated insult patch test. No evidence of irritation was seen.

Respiratory Sensitization (SnR) Group II* Score (H, M, or L): DG

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite were assigned a score of Data Gap for respiratory sensitization based on a lack of data for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists
- No data were identified for this endpoint.

Skin Irritation/Corrosivity (IrS) Group II Score (vH, H, M, or L): L

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite were assigned a score of Low for skin irritation/corrosivity based on dermal irritation studies in rabbits for another organoclay compound. GreenScreen® criteria classify chemicals as a Low hazard for skin irritation/corrosivity when adequate data are available and are negative for dermal irritation, and the chemical is not present on authoritative or screening lists (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists

<u>Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 71011-24-0)</u>

- No data were identified for this endpoint.

<u>Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 68953-58-2)</u>

- OECD 2008b
  - Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite were not irritating in a GLP-compliant dermal irritation test according to FHSLA 16 CFR 1500.41. Six rabbits (sex and strain not specified) were dermally administered 0.5 g undiluted quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite to clipped skin for 24 hours under occlusion. Sites were wiped clean after 24 hours and were evaluated at 24 and 72 hours. No erythema or edema was noted.
  - Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite were not irritating in a GLP-compliant modified Draize test. Six New Zealand white rabbits were dermally administered 0.5g undiluted quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite to abraded and intact skin for 24 hours under occlusion . No signs of erythema or edema were seen after 24 or 72 hours.
  - Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite were not irritating in a second dermal irritation test according to FHSLA 16 CFR 1500.41. Six rabbits (sex and strain not specified) were dermally administered 0.5 g undiluted quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite to clipped intact and abraded skin for 24 hours under occlusion. Sites were

wiped clean after 24 hours and were evaluated at 24 and 72 hours. No erythema or edema was noted in any of the animals.
- Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite was not irritating when administered undiluted to the depilitated intact and abraded skin of 10 rabbits for 10 days. No edema, erythema, or eschar was observed (All Draize scores were 0). No additional details were provided.

Eye Irritation/Corrosivity (IrE) Group II Score (vH, H, M, or L): *M*
Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite were assigned a score of Moderate for eye irritation/corrosivity based on an ocular irritation study in rabbits. GreenScreen® criteria classify chemicals as a Moderate hazard for eye irritation/corrosivity when available data indicate classification as GHS Category 2 (mildly irritating) (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists

<u>Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 71011-24-0)</u>

- No data were identified for this endpoint.

<u>Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 68953-58-2)</u>

- OECD 2008b
  - Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite were not irritating in a GLP compliant ocular irritation test according to FHSLA 16 CFR 1500.42 in six rabbits (sex and strain not specified). The test substance (0.1 mL) was administered to the everted lower eyelid of one eye without washing, and lesions were scored at 24, 48, and 72 hours. No signs of irritation were observed.
  - Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite were not irritating in a second ocular irritation test according to FHSLA 16 CFR 1500.42 in six rabbits (sex and strain not specified). The test substance (0.1 g) was administered to the everted lower eyelid of one eye without washing, and lesions were scored at 24, 48, and 72 hours. No corneal, iridial, or conjunctival irritation was observed.
  - Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite were not irritating when a 10% solution in saline was administered to the eyes of 10 rabbits (sex and strain not specified). The cornea, iris and conjunctiva were negative for irritation (time of observation not specified). No additional details were provided.
  - Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite was moderately irritating in a GLP compliant ocular irritation test using modified Draize procedures test in six New Zealand white rabbits. The undiluted test substance (0.1g) was administered into one eye without washing. Draize scores at 24, 48, and 72 hours, and 4 and 7 days were 36.0, 23.7, 12.8, 14.2, and 4.0, respectively. Authors considered the substance to be a moderate irritant.
- Based on the weight of evidence, a score of Moderate was assigned. Most studies demonstrate no ocular irritation following administration of quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite, but in one GLP-compliant ocular irritation study, authors reported moderate irritation. While the scoring scale in this study is different from that used in the OECD Guideline 405 test recommended by GHS guidance, authors describe moderate irritation that is apparently reversible within 7 days, which best corresponds to GHS Category 2b. Therefore, a

conservative score of Moderate was assigned based on the results of this study. Confidence in this score is reduced due to conflicting results between studies.

Ecotoxicity (Ecotox)

Acute Aquatic Toxicity (AA) Score (vH, H, M, or L): L

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite was assigned a score of Low for acute aquatic toxicity based on LC/EC_{50} values for quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite and other organoclay compounds. GreenScreen® criteria classify chemicals as a Low hazard for acute aquatic toxicity when acute aquatic toxicity values are greater than 100 mg/L. (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with bentonite (CAS# 71011-24-0)

- OECD 2007
  - 96-hour LC_{50} (*Oncorhynchus mykiss*) = greater than 500 mg/L

Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 68953-58-2)

- OECD 2008b
  - 48-hour EC_{50} (*Daphnia magna*) = greater than 100 mg/L
  - 96-hour LC_{50} (*Americamysis bahia*) = greater than 1,000,000 mg/L
  - 48-hour EC_{50} (*Acartia tonsa*) = greater than 2,000 mg/L
  - 72-hour EC_{50} (*Skeletonema costatum*) = greater than 1,000 mg/L

Quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, salts with hectorite (CAS# 121888-67-3)

- OECD 2007
  - 96-hour LC_{50} (*Oncorhynchus mykiss*) = greater than 500 mg/L

Chronic Aquatic Toxicity (CA) Score (vH, H, M, or L): M

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite was assigned a score of Moderate for chronic aquatic toxicity based on a 21-day LOEC for reproduction in *Daphnia magna*. GreenScreen® criteria classify chemicals as a Moderate hazard for chronic aquatic toxicity when chronic aquatic toxicity values are greater than 1.0-10 mg/L (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)methyl, salts with hectorite (CAS# 121888-67-3)

- OECD 2007
  - 21-day reproduction NOEC (*Daphnia magna*) = 3.2 mg/L; LOEC = 10 mg/L; EC_{50} = 7.6 mg/L

Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 68953-58-2)

- OECD 2008b
  - 72-hour NOEC (*Skeletonema costatum*) = 100 mg/L

Environmental Fate (Fate)

Persistence (P) Score (vH, H, M, L, or vL): *vH*

Quaternary ammonium compounds, benyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite were assigned a score of Very High for persistence based on biodegradation data and expert judgment. GreenScreen® criteria classify chemicals as a Very High hazard for persistence when the chemical is expected to be recalcitrant (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists

Organoclay compounds

- OECD 2007
  - Organoclay compounds are not considered biodegradable due to low organic content. In the environment, hydrophobic organoclay will initially float on the water surface but over time will settle into the sediment, where the organic components are susceptible to biodegradation and the clay component will remain in the sediment.

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with bentonite (CAS# 71011-24-0)

- OECD 2007
  - In three biodegradation tests according to OECD Guideline 306 (Biodegradability in Seawater), quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with bentonite achieved 3.3-33.4% biodegradation in 28 days.
- Grabinska-Sota 2011
  - Quaternary ammonium salts were studied for their biodegradation in the aquatic environments. Although the rate of biodegradation is influenced by the hydrocarbon chain length, the presence of aromatic or cyclic rings and the occurrence of sulphur and oxygen atoms in the alkyl substituent, the half-life of the different quaternary ammonium salts ranged from 0.5-1.6 days.
- Based on the weight of evidence, a score of Very High was assigned. Biodegradation is only applicable to the organic components of organoclay compounds. As indicated by the biodegradation studies above, the quaternary ammonium moiety of organoclays are expected to be biodegradable. While the clay moiety is expected to be recalcitrant. Therefore, the score for this endpoint is based on the property of the inorganic moiety. Confidence in this score is reduced as no data on the half-lives for organoclay compounds are available.

Bioaccumulation (B) Score (vH, H, M, L, or vL): *L*

Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite were assigned a score of Low for bioaccumulation based on the low likelihood of bioaccumulation for a chemical with its physicochemical properties. GreenScreen® criteria classify chemicals as a Low hazard for bioaccumulation when the chemical is not expected to bioaccumulate (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* DSL: DSL Substances that are Bioaccumulative
- No data were identified.
- OECD 2007
  - Organoclays are insoluble in water, organic solvents, and lipids. Therefore, a partition coefficient is not applicable.

- Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite was classified as Bioaccumulative by Environment Canada's DSL. However, it is unclear why is it classified as bioaccmulative and no data were identified to support this classification. Based on its low solubility in lipids and in water, ToxServices considered that this substance is not likely to be bioaccumulative, as it cannot be taken up by cells. Organoclays are not expected to be absorbed even after ingestion, and there is no evidence of tissue retention or systemic uptake of these compounds (OECD 2007). As this assessment was based on expert judgment without measured BCF/BAF data, the score is italicized.

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M, or L): L
Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite was assigned a score of Low for reactivity based on not being inherently explosive or having oxidizing properties. GreenScreen® criteria classify chemicals as a Low hazard for reactivity when the chemical is not GHS classified as explosive or an oxidizer (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists
- OECD 2007
  - Organoclays are not inherently explosive.
  - Organoclays are not oxidizers.

Flammability (F) Score (vH, H, M, or L): L
Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite was assigned a score of Low for flammability based data from another organoclay compound indicating it does not burn and is not flammable based on its HMIS score for flammability. GreenScreen® criteria classify chemicals as a Low hazard for flammability when data indicate that the chemical is not GHS classified for flammability.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists

Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite (CAS# 68953-58-2)

- ESIS 2000
  - Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite ignite at 370°C with rapid extinction.
- Zhejiang undated
  - Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite received an HMLS code of 0 for flammability, which indicates "Will Not Burn: substance that will not burn" (Oklahoma State Undated).

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APPENDIX A: Hazard Benchmark Acronyms
(in alphabetical order)

(AA) Acute Aquatic Toxicity

(AT) Acute Mammalian Toxicity

(B) Bioaccumulation

(C) Carcinogenicity

(CA) Chronic Aquatic Toxicity

(D) Developmental Toxicity

(E) Endocrine Activity

(F) Flammability

(IrE) Eye Irritation/Corrosivity

(IrS) Skin Irritation/Corrosivity

(M) Mutagenicity and Genotoxicity

(N) Neurotoxicity

(P) Persistence

(R) Reproductive Toxicity

(Rx) Reactivity

(SnS) Sensitization- Skin

(SnR) Sensitization- Respiratory

(ST) Systemic/Organ Toxicity

APPENDIX B: Results of Automated GreenScreen® Score Calculation for Quaternary Ammonium Compounds, Benzyl(hydrogenated tallow alkyl)dimethyl, Salts with Bentonite (CAS #71011-24-0)

TOXSERVICES TOXICOLOGY RISK ASSESSMENT CONSULTING

GREEN SCREEN FOR SAFER CHEMICALS

GreenScreen® Score Inspector

Table 1: Hazard Table

			Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
			Carcinogenicity	Mutagenicity/Genotoxicity	Reproductive Toxicity	Developmental Toxicity	Endocrine Activity	Acute Toxicity	Systemic Toxicity		Neurotoxicity		Skin Sensitization*	Respiratory Sensitization*	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Reactivity	Flammability
Table 2: Chemical Details									S	R *	S	R *	*	*								
Inorganic Chemical?	**Chemical Name**	**CAS#**	**C**	**M**	**R**	**D**	**E**	**AT**	**STs**	**STr**	**Ns**	**Nr**	**SNS***	**SNR***	**IrS**	**IrE**	**AA**	**CA**	**P**	**B**	**Rx**	**F**
No	Quaternary Ammonium Compounds, benzyl(Hydrogenated Tallow alkyl)Dimethyl, Salts with Bentonite	**71011-24-0**	*L*	**L**	**L**	**L**	DG	**L**	**L**	**L**	DG	DG	**L**	DG	**L**	*M*	**L**	**M**	*vH*	*L*	**L**	**L**

Table 3: Hazard Summary Table

Benchmark	a	b	c	d	e	f	g
1	No	No	No	No	No		
2	No	No	Yes	No	No	No	No
3	STOP						
4	STOP						

Table 4

Chemical Name	Preliminary GreenScreen® Benchmark Score
Quaternary Ammonium Compounds, benzyl(Hydrogenated Tallow alkyl)Dimethyl, Salts with Bentonite	2

Note: Chemical has not undergone a data gap assessment. Not a Final GreenScreen™ Score

Table 6

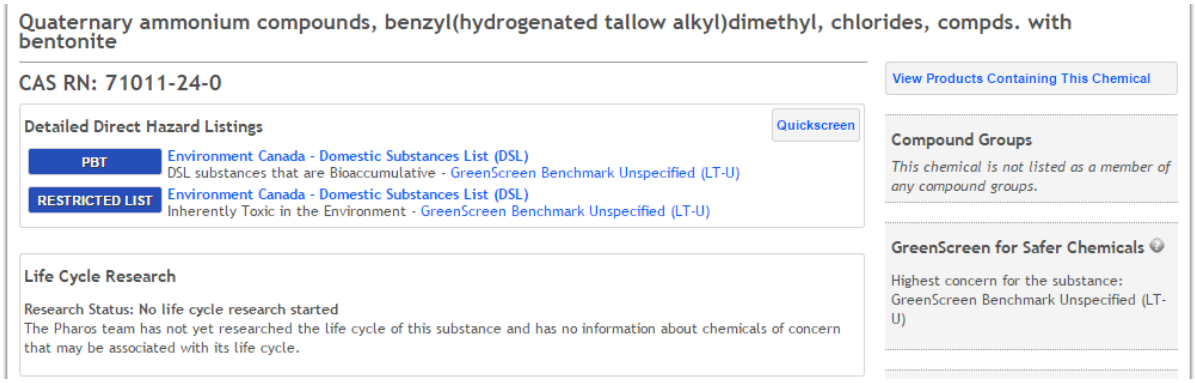
Chemical Name	Final GreenScreen® Benchmark Score
Quaternary Ammonium Compounds, benzyl(Hydrogenated Tallow alkyl)Dimethyl, Salts with Bentonite	2

After Data gap Assessment
Note: No Data gap Assessment Done if Preliminary GS Benchmark Score is 1.

Table 5: Data Gap Assessment Table

Datagap Criteria	a	b	c	d	e	f	g	h	i	j	bm4	End Result
1												
2	Yes	Yes	Yes	Yes	Yes							2
3												
4												

APPENDIX C: Pharos Output for Quaternary Ammonium Compounds, Benzyl(hydrogenated tallow alkyl)dimethyl, Salts with Bentonite (CAS# 71011-24-0)



Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compds. with bentonite

CAS RN: 71011-24-0

View Products Containing This Chemical

Detailed Direct Hazard Listings

Quickscreen

PBT — Environment Canada - Domestic Substances List (DSL)
DSL substances that are Bioaccumulative - GreenScreen Benchmark Unspecified (LT-U)

RESTRICTED LIST — Environment Canada - Domestic Substances List (DSL)
Inherently Toxic in the Environment - GreenScreen Benchmark Unspecified (LT-U)

Compound Groups

This chemical is not listed as a member of any compound groups.

GreenScreen for Safer Chemicals

Highest concern for the substance: GreenScreen Benchmark Unspecified (LT-U)

Life Cycle Research

Research Status: No life cycle research started
The Pharos team has not yet researched the life cycle of this substance and has no information about chemicals of concern that may be associated with its life cycle.

Sources to Check for GreenScreen® Hazard Assessment

Note: For a GreenScreen® Hazard Assessment, data queries should be initially limited to the following references. If data gaps exist after these references have been checked, additional references may be utilized.

U.S. EPA High Production Volume Information System (HPVIS):
http://www.epa.gov/hpvis/index.html

UNEP OECD Screening Information Datasets (SIDS):
http://www.chem.unep.ch/irptc/sids/OECDSIDS/sidspub.html

OECD Existing Chemicals Database: http://webnet.oecd.org/hpv/ui/SponsoredChemicals.aspx

European Chemical Substances Information System IUCLID Chemical Data Sheets:
http://esis.jrc.ec.europa.eu/index.php?PGM=dat

National Toxicology Program: http://ntp.niehs.nih.gov/

International Agency for the Research on Cancer:
http://monographs.iarc.fr/ENG/Classification/index.php

Human and Environmental Risk Assessment (HERA) on ingredients of household cleaning products:
http://www.heraproject.com/RiskAssessment.cfm

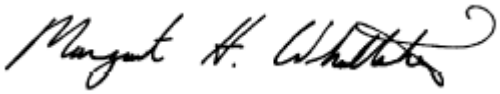
European Chemicals Agency (ECHA) REACH Dossiers: http://echa.europa.eu/

Licensed GreenScreen® Profilers

Quaternary Ammonium Compounds, Benzyl(hydrogenated tallow alkyl)dimethyl, Salts with Bentonite GreenScreen® Evaluation Prepared by:

Sara M. Ciotti, Ph.D.
Toxicologist
ToxServices LLC

Quaternary Ammonium Compounds, Benzyl(hydrogenated tallow alkyl)dimethyl, Salts with Bentonite GreenScreen® Evaluation QC'd by:



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