TSCA Section 5(a)(3) Determination for Premanufacture Notice (PMN) P-16-0400

PMN Number: P-16-0400
TSCA Section 5(a)(3) Determination: The chemical substance is not likely to present an unreasonable risk (5(a)(3)(C))

Chemical Name:
Specific: Alkanes, C11-16-branched and linear; CASRN: 1809170-78-2

Conditions of Use (intended, known, or reasonably foreseen)[1]:
Intended conditions of use (specific): Import at an estimated maximum production volume of 63,500,000 kg/year for processing for and use as a chemical intermediate (53.4%), solvent/diluent in coatings (25%), cleaning fluids (9.5%), metalworking fluids/rolling oils (8.9%), and in agrochemicals (3.2%), consistent with the manufacturing, processing, use, distribution, and disposal information described in the PMN.
Known conditions of use: Applying such factors as described in footnote 1, EPA evaluated whether there are known conditions of use and found none.
Reasonably foreseen conditions of use: Applying such factors as described in footnote 1, EPA evaluated whether there are reasonably foreseen conditions of use and identified consumer use as a reasonably foreseen condition of use.

Summary: The chemical substance is not likely to present an unreasonable risk of injury to health or the environment, without consideration of costs or other nonrisk factors, including an unreasonable risk to a potentially exposed or susceptible subpopulation identified as relevant by the Administrator under the conditions of use, based on the risk assessment presented below. Although EPA estimated that the new chemical substance could be persistent, and the new chemical substance has low to moderate potential for bioaccumulation, the chemical substance is expected to have low chronic toxicity. Based on EPA's TSCA New Chemicals Program Chemical Categories for Neutral Organics[2] and test data on analogous chemical substances, EPA estimates that the chemical substance has low environmental hazard and the potential for the

[1] Under TSCA § 3(4), the term "conditions of use" means "the circumstances, as determined by the Administrator, under which a chemical substance is intended, known, or reasonably foreseen to be manufactured, processed, distributed in commerce, used, or disposed of." In general, EPA considers the intended conditions of use of a new chemical substance to be those identified in the section 5(a) notification. Known conditions of use include activities within the United States that result from manufacture that is exempt from PMN submission requirements. Reasonably foreseen conditions of use are future circumstances, distinct from known or intended conditions of use, under which the Administrator expects the chemical substance to be manufactured, processed, distributed, used, or disposed of. The identification of "reasonably foreseen" conditions of use will necessarily be a case-by-case determination and will be highly fact-specific. Reasonably foreseen conditions of use will not be based on hypotheticals or conjecture. Accordingly, EPA will apply its professional judgment, experience, and discretion when considering such factors as evidence of current use of the new chemical substance outside the United States, evidence that the PMN substance is sufficiently likely to be used for the same purposes as existing chemical substances that are structurally analogous to the new chemical substance, and conditions of use identified in an initial PMN submission that the submitter omits in a revised PMN. The sources EPA uses to identify reasonably foreseen conditions of use include searches of internal confidential EPA PMN databases (containing use information on analogue chemicals), other U.S. government public sources, the National Library of Medicine's Hazardous Substances Data Bank (HSDB), the Chemical Abstract Service STN Platform, REACH Dossiers, technical encyclopedias (e.g., Kirk-Othmer and Ullmann), and Internet searches.
[2] TSCA New Chemicals Program (NCP) Chemical Categories. https://www.epa.gov/reviewing-new-chemicals-under-toxic-substances-control-act-tsca/chemical-categories-used-review-new.

following human health hazards: dermal irritation and lung toxicity if aerosols were inhaled. EPA concludes that the new chemical substance is not likely to present an unreasonable risk under the conditions of use.

Fate: Environmental fate is the determination of which environmental compartment(s) a chemical moves to, the expected residence time in the environmental compartment(s) and removal and degradation processes. Environmental fate is an important factor in determining exposure and thus in determining whether a chemical may present an unreasonable risk. EPA estimated physical/chemical and fate properties of this new chemical substance using EPI (Estimation Programs Interface) Suite, a suite of physical/chemical property and environmental fate estimation programs (http://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface). The chemical substance is estimated to be removed during wastewater treatment with an efficiency of 90% via sorption, biodegradation, and stripping, depending on chain length and branching. Sorption to sludge, soil, and sediment is estimated to be moderate to strong, resulting in slow to moderate migration to groundwater. Volatilization to air is estimated to be negligible to moderate based on the estimated vapor pressure and Henry's Law constant of the new chemical substance. Overall, these estimates are indicative of low to moderate potential for this chemical substance to volatilize into the air and a low to moderate potential for this chemical substance to migrate into groundwater.

Persistence[3]: Persistence is relevant to whether a new chemical substance is likely to present an unreasonable risk because chemicals that are not degraded in the environment at rates that prevent substantial buildup in the environment, and thus increase potential for exposure, may present a risk if the substance presents a hazard to human health or the environment. EPA estimated biodegradation half-lives of this new chemical substance using EPI (Estimation Programs Interface) Suite, a suite of physical/chemical property and environmental fate estimation programs (http://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface). EPA estimates the aerobic and anaerobic biodegradation half-lives to be from less than 2 months up to six months, depending on the chain length and branching. These estimates for biodegradation indicate that components of the new chemical substsance may be persistent in aerobic environments (e.g., surface water) and anaerobic environments (e.g., sediment).

Bioaccumulation[4]: Bioaccumulation is relevant to whether a new chemical substance is likely to present an unreasonable risk because substances that bioaccumulate in aquatic and/or terrestrial species pose the potential for elevated exposures to humans and other organisms via

---

[3] Persistence: A chemical substance is considered to have limited persistence if it has a half-life in water, soil or sediment of less than 2 months or there are equivalent or analogous data. A chemical substance is considered to be persistent if it has a half-life in water, soil or sediments of greater than 2 months but less than or equal to 6 months or if there are equivalent or analogous data. A chemical substance is considered to be very persistent if it has a half-life in water, soil or sediments of greater than 6 months or there are equivalent or analogous data. (64 FR 60194; November 4, 1999)

[4] Bioaccumulation: A chemical substance is considered to have a low potential for bioaccumulation if there are bioconcentration factors (BCF) or bioaccumulation factors (BAF) of less than 1,000 or there are equivalent or analogous data. A chemical substance is considered to be bioaccumulative if there are BCFs or BAFs of 1,000 or greater and less than or equal to 5,000 or there are equivalent or analogous data. A chemical substance is considered to be very bioaccumulative if there are BCFs or BAFs of 5,000 or greater or there are equivalent or analogous data. (64 FR 60194; November 4 1999)

food chains. EPA estimated the potential for the new chemical substance to bioaccumulate using EPI (Estimation Programs Interface) Suite, a suite of physical/chemical property and environmental fate estimation programs (http://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface). The new chemical substance is expected to have low to moderate bioaccumulation potential based bioconcentration and bioaccumulation factors of less than 1000 to greater than 1000 depending on chain length and degree of branching. However, potential bioaccumulation in food chains is not expected to result in effects due to low hazard of the new chemical substance.

Human Health Hazard[5]: Human health hazard is relevant to whether a new chemical substance is likely to present an unreasonable risk because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated the human health hazard of this chemical substance based on its estimated physical/chemical properties, data on analogous chemicals identified by EPA and the PMN submitter in the Sustainable Futures submission, and structural information. Absorption of the low molecular weight components of the new chemical substance is expected to be poor via all routes of exposure, based on physical/chemical properties. EPA identified dermal irritation hazard for the low molecular weight components based on *in vitro* and *in vivo* skin irritation test data for C8-C11 and C9-C12 hydrocarbons. EPA quantitatively assessed risk for lung effects using test data for C20-C50 hydro-treated oil. EPA identified a NOEC of 1000 mg/m3 (highest aerosol concentration tested) in a 28-day Inhalation Toxicity Study (similar to OECD 412)[6], which was used to derive exposure route- and population-specific points of departure for quantitative risk assessment, described below.

Environmental Hazard[7]: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risk because the significance of the risk is dependent

[5] A chemical substance is considered to have low human health hazard if effects are observed in animal studies with a No Observed Adverse Effect Level (NOAEL) equal to or greater than 1,000 mg/kg/day or if there are equivalent data on analogous chemical substances; a chemical substance is considered to have moderate human health hazard if effects are observed in animal studies with a NOAEL less than 1,000 mg/kg/day or if there are equivalent data on analogous chemical substances; a chemical substance is considered to have high human health hazard if there is evidence of adverse effects in humans or conclusive evidence of severe effects in animal studies with a NOAEL of less than or equal to 10 mg/kg/day or if there are equivalent data on analogous chemical substances. EPA may also use Benchmark Dose Levels (BMDL) derived from benchmark dose (BMD) modeling as points of departure for toxic effects. See https://www.epa.gov/bmds/what-benchmark-dose-software-bmds. Using this approach, a BMDL is associated with a benchmark response, for example a 5 or 10 % incidence of effect. The aforementioned characterizations of hazard (low, medium, high) would also apply to BMDLs. In the absence of animal data on a chemical or analogous chemical substance, EPA may use other data or information such as from in vitro assays, chemical categories (e.g., Organization for Economic Co-operation and Development, 2014 Guidance on Grouping of Chemicals, Second Edition. ENV/JM/MONO(2014)4. Series on Testing & Assessment No. 194. Environment Directorate, Organization for Economic Co-operation and Development, Paris, France. (http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono(2014)4&doclanguage=en)), structure-activity relationships, and/or structural alerts to support characterizing human health hazards.

[6] CoCAM 1, 10-12 October 2011, C14-C20 Aliphatic [≤2% aromatic] Hydrocarbon Solvents category, SIDS Initial Assessment Profile.

[7] A chemical substance is considered to have low ecotoxicity hazard if the Fish, Daphnid and Algae LC50 values are greater than 100 mg/L, or if the Fish and Daphnid chronic values (ChVs) are greater than 10.0 mg/L, or there are not effects at saturation (occurs when water solubility of a chemical substance is lower than an effect concentration), or the log Kow value exceeds QSAR cut-offs. A chemical substance is considered to have moderate ecotoxicity hazard

upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated acute hazard for the low molecular weight species (MW 156.21; n-undecane, CASRN 1120-21-4) for this new chemical substance using the Ecological Structure Activity Relationships (ECOSAR) Predictive Model (https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-releationships-ecosar-predictive-model); specifically, the QSAR for the class of neutral organics. EPA estimated chronic environmental hazard of this new chemical substance using data on analogous chemical substance. Hazards from acute and chronic exposures are not expected at concentrations up to the water solubility limit of the new chemical substance (i.e., no effects at saturation). The toxicity values for both the new chemical substance and the low molecular weight species indicate the chemical substance is expected to have low hazard. Because hazards are not expected up to the water solubility limit, acute and chronic concentrations of concern are not identified.

Exposure: The exposure to a new chemical substance is potentially relevant to whether a new chemical substance is likely to present unreasonable risks because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance.

EPA estimates occupational exposure and environmental release of the new chemical substance under the intended conditions of use described in the PMN using ChemSTEER (Chemical Screening Tool for Exposures and Environmental Releases https://www.epa.gov/tsca-screening-tools/chemsteer-chemical-screening-tool-exposures-and-environmental-releases). EPA uses EFAST (the Exposure and Fate Assessment Screening Tool; https://www.epa.gov/tsca-screening-tools/e-fast-exposure-and-fate-assessment-screening-tool-version-2014) to estimate general population, consumer, and environmental exposures.

EPA considers workers to be a potentially exposed or susceptible subpopulation (PESS) on the basis of greater exposure potential compared to the general population. EPA also considers PESS in conducting general population drinking water exposures by evaluating risks associated with water intake rates for multiple age groups, ranging from infants to adults. EPA considers consumers of specific products to be a potentially exposed or susceptible subpopulation on the basis of greater exposure potential compared to the general population who do not use specific products.

For this new chemical assessment, EPA assessed exposure to workers via the dermal and inhalation routes. Exposure to the general population was assessed via inhalation. Exposure to the general population via drinking water was not assessed because releases to water were below modeling thresholds. Although consumer use was not identified as an intended use, it was identified as a reasonable foreseen condition of use, and potential consumer exposures were

---

if the lowest of the Fish, Daphnid or Algae LC50s is greater than 1 mg/L and less than 100 mg/L, or where the Fish or Daphnid ChVs are greater than 0.1 mg/L and less than 10.0 mg/L. A chemical substance is considered to have high ecotoxicity hazard, or if either the Fish, Daphnid or Algae LC50s are less than 1 mg/L, or any Fish or Daphnid ChVs is less than 0.1 mg/L (Sustainable Futures https://www.epa.gov/sustainable-futures/sustainable-futures-p2-framework-manual).

assessed as a hypothetical scenario using a model for general purpose cleaner, latex paint, and laundry detergent.

Risk Characterization: EPA applies a margin of exposure approach to calculate potential human health risks of new chemicals. A benchmark (acceptable) margin of exposure is derived by applying uncertainty factors for the following types of extrapolations: intra-species extrapolation (UF_H = 10 to account for variation in sensitivity among the human population), inter-species extrapolation (UF_A = 10 to account for extrapolating from experimental animals to humans) and LOAEL-to-NOAEL extrapolation (UF_L = 10 to account for using a LOAEL when a NOAEL is not available). Hence, in the New Chemicals Program, a benchmark MOE is typically 100 and 1000 when NOAELs (i.e., NOECs) and LOAELs, respectively, are used to identify hazard. When allometric scaling or pharmacokinetic modeling is used to derive an effect level, the UF_H may be reduced to 3, for a benchmark MOE of 30. The benchmark MOE is used to compare to the MOE calculated by comparing the toxicity NOAEL or LOAEL to the estimated exposure concentrations. When the calculated MOE is equal to or exceeds the benchmark MOE, the new chemical substance is not likely to present an unreasonable risk. EPA assesses risks to workers considering engineering controls described in the PMN but in the absence of personal protective equipment (PPE) such as gloves and respirators. If risks are preliminarily identified, EPA then considers whether the risks would be mitigated by the use of PPE (e.g., impervious gloves, respirator).

Risks to human health for the new chemical substance were evaluated using the route-specific effect levels (i.e., NOEC) described above. Risks were not identified for workers from inhalation exposures because the MOE (MOE = 160) exceeded the benchmark MOE of 100. Dermal irritation to workers was identified as a hazard but not quantified due to a lack of dose-response for this hazard. However, exposures will be controlled by the use of appropriate PPE, including impervious gloves. EPA expects that workers will use appropriate PPE consistent with the Safety Data Sheet prepared by the PMN submitter, in a manner adequate to protect them.

Risks were not identified for the general population or consumers from inhalation exposures because the MOEs ($MOE_{general\ population}$ =7.3E+3, $MOE_{consumers}$ =7.3E+3) exceeded the benchmark MOE of 100.

Risks to the environment were not identified based on no effects expected at the limit of solubility of the new chemical substance.

Because worker exposures can be controlled by PPE, no unreasonable risks to the general population, consumers, or environment were identified, EPA has determined that the new chemical substance is not likely to present unreasonable risk to human health or the environment under the conditions of use.

12/21/18
Date:

/s/
Jeffery T. Morris, Director
Office of Pollution Prevention and Toxics