5/6/2020 DS
10/1/2020 JS

Chemistry Report for Case # P-19-0134

General

Submitter: [redacted]

Contact: Jeff Laikind

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TS No.: AfFW19

Chemist: Yakal, R.

Contractor Support: Y

PV Init (kg/yr): 80000.0

PV Max (kg/yr): 600000.0

Binding Option: ☐

Exposure-Based Review: [redacted]

Manufacture: ☑

Import: ☐

CAS Number: None

Chemical Name: [redacted]

Trade Name: Affinity

IES Order: None

Generic Name: 5-Isocyanato-1-(isocyanatomethyl)-1,3,3-trimethylcyclohexane, poly[oxy(methyl-1,2-ethanediyl)], .alpha.-hydro-.omega.-hydroxy-, polymer with 1,6-diisocyanatohexane, polymer with poly(oxy-1,4-butanediyl), .alpha.-hydro-.omega.-hydroxy-, cyclic amine - ketone adduct, reduced, and 1,3-propanediol, 2-ethyl-2-(hydroxymethyl)-

Chemical Structure

[redacted]

Physical Chemical Properties

Molecular Formula:[redacted]	**Molecular Weight:**6100.0
% < 500:0.1	**% < 1000:**13.3
MP:	**MP Estimate:**
BP:	**BP Pressure:**
BP Estimate:>400	
VP (Torr):	**VP Estimate (Torr):**<0.000001
Water Solubility (g/L):	**Water Soluble Estimate (g/L):**Reacts
Log P:	**Log P Estimate:**
Physical State — Neat: Solid (est.)	**Physical State — Manuf:**Solution: 80% PMN substance in xylene and 2-heptanone

Physical State — Processing: Solution or Dispersion: 40-50% PMN substance in coating formulation
Physical State — End Use: Destroyed

Additional Chemical Info

NAVG
MW = 6100 with 0.10% < 500 and 13.30% < 1000 by submitter estimation based on molecular weights and molar ratios of feedstocks.
Submitted
Data: The two submitted MSDSs are for the isocyanate feedstock [redacted] and a formulation of the PMN substance. An IR spectra was included in the submission.
Isocyanate FGEW = 6100/3 = 2030 (three terminal groups in structure as drawn).
Estimated Data: BP> 400 (Polymer); VP < 0.000001 torr (Polymer); The substance will hydrolyze slowly (days-weeks) by reaction of the terminal isocyanate groups to yield a polymer bearing terminal NH2 groups.

Uses

Consumer Use? No

Use:	Intended use: Isocyanate binder resin for white reflective moisture-cure roofing coatings. Isocyanate FGEW = 2030. Same as case L-11-0297 [redacted] is for the same use. Analogues (Same Use): All analogues [redacted] Patents (same use): None found.
Other Uses:	Analogues (other uses): None found. Analogues (same + other uses): None found. Patents (other uses): None found.

Reaction Description

Cyclohexane,
5-isocyanato-1-(isocyanatomethyl)-1,3,3-trimethyl-; and

poly[oxy(methyl-1,2-ethanediyl)], .alpha.-hydro-.omega.-hydroxy-, polymer with 1,6-diisocyanatohexane are added to a reactor under a nitrogen blanket, along with xylene, 2-heptanone, and dibutyltin dilaurate. The reactor is heated to 50°C, with mixing. Poly(oxy-1,4-butanediyl), .alpha.-hydro-.omega.-hydroxy-; and 1,3-propanediol, 2-ethyl-2-(hydroxymethyl)- are mixed together with xylene and heated to 40°C, then loaded into the reactor, forming a polymeric intermediate after mixing at 60-70°C for 30-90 minutes. The reactor is cooled to 26°C. 2-Propanone, reaction products with 5-amino-1,3,3-trimethylcyclohexanemethanamine, reduced is loaded last, and the reaction takes place at 25-30Â°C over 30-90 minutes to form the PMN substance. The substance in xylene and 2-heptanone is transferred to a mixing tank, into which rheology additives, a catalyst, UV stabilizer, pigments, moisture scavengers, defoamer, and additional xylene are added.

Pollution Prevention Analysis(P2 Analysis:)

P2
Claims: This chemical, an aliphatic polyisocyanate, is to be manufactured for moisture cured coatings. The primary use is for white roof coatings applied on flat industrial roofs to achieve high reflectivity and reduced cooling costs, saving energy. The coating will be registered with Energy Star and the Cool Roof Rating Council for energy savings. The polymers typically used for this application have certain drawbacks that are addressed by this chemical. Polymers currently used are: 1) Aromatic polyurethanes. These polymers are degraded by ultraviolet light, leading to chalking and eventual disintegration of the coating. Coatings made from this chemical have high resistance to ultraviolet light, leading to improved durability and longer application life. 2) Silicone polymers. Due to the surface energy of these polymers, particulates are electrostatically attracted to the coating, resulting in lower solar reflectance. Coatings made from this chemical do not have the electrostatic attraction, and will remain cleaner, leading to improved solar reflectance over time. 3) Elastomeric acrylic latexes. These coatings soften when heated by sunlight, allowing dirt to physically attach to the surface, reducing reflectivity. As the reflectivity drops, the coatings absorb more sunlight, which softens the coating more, allowing more dirt to bond to the surface. This pattern repeats until the coating is completely obscured and the solar reflectance drops to 0. Coatings made from this chemical are resistant to dirt, even when heated, resulting in higher solar reflectivity and longer application life.

Analogs

Same as L-11-0297. [redacted]

Comments/Telephone Log

Artifact	Update/Upload Time
[redacted]	[redacted]