Fate Report for Case # P-22-0162 (Version 1)

Fate Summary Statement

Fate Summary Statement: P-22-0162
FATE Estimations for hydrolysis product
log Kow = -0.09 (E)
log Koc 0 00 (E)
log Fish BCF = 0.5 (3.2) (E)
log Fish BAF 0 03 (0 9) (E)
PMN Substance: Solid with MP = 33 °C (M)
S Reacts
Hydrolysis Half-life = min
VP 1 0E 6 torr at 25 °C (E)
BP = 236 °C (NOMO5) based on 113 °C @ 13 mm Hg (M)
H 1 00E 8 (E)
POTW removal (%) = PMN 99 via hydrolysis; then Hyd Pdt 95 via biodeg; OECD 111
(Hydrolysis): hydrolysis occurred rapidly (pH 4,7,9) @ 50C;
OECD 111 (Hydrolysis) t1/2 (pH 4,7,9) 1h/ 1h/ 1h @ 15 0C;
OECD 301B (Mod Sturm CO2 ev): 89.3%/28d, RB.
Time for complete ultimate aerobic biodeg Hyd Pdt wk
Sorption to soils/sediments = Hyd Pdt low
PBT Potential PMN P1B1; Hyd Pdt P1B1
FATE: Migration to ground water = PMN negl; Hyd Pdt negl
Bioconcentration factor to be put into E FAST PMN N/A; Hyd Pdt 3

Analog data found (include identifier and database) [redacted]
(ECHA) [redacted] (ECHA and Jcheck)
Relevant Structure(s)
Water Hydrolysis product(s)
Landfill Hydrolysis product(s)
Air / Incineration Parent
Parent % Incineration 99.9%

Environmental Fate Determination

PMN #: P-22-0162
Summary EPA estimated that the new chemical substance and the hydrolysis product could have limited persistence and low potential for bioaccumulation, such that repeated exposures are not expected

to cause food chain effects via accumulation in exposed organisms

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 the new chemical substance using data submitted for the new chemical substance and of the hydrolysis product using data submitted for the new chemical substance and EPI (Estimation Program Interface) Suite™ (http //www epa gov/tsca screening tools/epi suitetm estimation-program-interface). In wastewater treatment, the new chemical substance is expected to be removed with an efficiency of 99% due to rapid hydrolysis and the hydrolysis product is expected to be removed with an efficiency of 95% due to biodegradation Removal of the hydrolysis product by biodegradation is high. Sorption of the hydrolysis product to sludge, soil and sediment is low. Migration of the new chemical substance to groundwater is expected to be negligible due to rapid hydrolysis and migration of the hydrolysis product to groundwater is expected to be negligible due to biodegradation Due to low estimated vapor pressure and Henry's law constant, the new chemical substance and the hydrolysis product are expected to undergo negligible volatilization to air. Overall, these estimates indicate that the new chemical substance and the hydrolysis product have low potential to volatilize to air and low potential to migrate to groundwater.

Persistence : 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 degradation half-lives of the new chemical substance using data submitted for the new chemical substance EPA estimated that the new chemical substance's hydrolysis half-life is minutes, and that the hydrolysis product's aerobic and anaerobic biodegradation half lives are < 2 months. These estimates indicate that the new chemical substance may have limited persistence in aerobic environments (e.g., surface water) and anaerobic environments (e g , sediments) due to hydrolysis Further, these estimates indicate that the hydrolysis product may have limited persistence in aerobic environments (e g , surface water) and anaerobic environments (e.g., sediment).

Bioaccumulation : 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 food chains. EPA estimated the potential for the new chemical substance to bioaccumulate using data submitted for the new chemical substance and of the hydrolysis product to bioaccumulate using EPI Suite™. EPA estimated that the new chemical substance has low bioaccumulation potential based on rapid hydrolysis and the hydrolysis product has low bioaccumulation potential based on BCFBAF model result < 1000 hydrolysis product bioconcentration factor = 3 [estimated by linear regression from log Kow] and bioaccumulation factor = 1 [estimated by the Arnot-Gobas method (2003)]). EPA estimated that the new chemical substance and the hydrolysis product could have limited persistence and low potential for bioaccumulation, such that repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms.

[redacted]

Fate Assessor: Moses, Sara

SMILES: [redacted]

Physical Properties

Property	Measured/Calculated Value	EPI
Molecular Form:	[redacted]	
Molecular Wt.:	144.56	
% < 500:		
% < 1000:		

Property	Measured Value	Method	Estimated Value	Method	EPI
Melting Point:	33				
Boiling Point:	118		236		
BP Pressure:	13.0				
Vapor Pressure:			0.049		
Water Solubility:			Reacts		
Log P:					
Log Kow:					
Log Koc:					
Log BCF:					
Henry's Law:					

pH:	
pH Comment:	

Fate Analysis

Hydrolysis (t1/2, da):	**Volatilization (t1/2) - River (hr):**	**Volatilization (t1/2) - Lake (da):**
Atm Ox Potential (t1/2)OH (hr):	**Atm Ox Potential (t1/2)O3 (hr):**	**Atm Ox Potential(t1/2) Total (hr):**
MITI Linear:	**MITI NonLinear:**	
Biodeg Linear:	**Biodeg NonLinear:**	
Biodeg Survey ult:	**Biodeg Survey Prim:**	
STP (% removal) Total:	**STP (% removal) Biodeg:**	
STP (% removal) Ads:	**STP (% removal) Air:**	

Rationales

Removal in Wastewater Treatment:	
Atmospheric Oxidation:	
Hydrolysis:	
Photolysis:	
Aerobic Biodegradation:	
Anaerobic Biodegradation:	
Sorption to Soil and Sediment:	
Migration to Groundwater:	

Persistence - Air:	
Persistence - Water:	
Volatilization from Water:	
Soil:	
Sediment:	
Other:	
Standard:	
Bioaccumulation:	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	PBT Comments
1	1		PMN
1	1		Hyd Pdt

Exposure-Based Testing

Exposure-Based Testing:

Fate Ratings

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
WWT/POTW Sorption:	;1	Low	Moderate	Strong	V. Strong	PMN;Hyd Pdt
WWT/POTW Stripping:	4;4	Extensive	Moderate	Low	Negligible	PMN;Hyd Pdt
Biodegradation Removal:	;2	Unknown	High	Moderate	Negligible	PMN;Hyd Pdt
Biodegradation Destruction:		Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	;2	Days	Weeks	Months	Months	PMN;Hyd Pdt
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
Anaerobic Biodeg Ult:	;2	<= Days	Weeks	Months	> Months	PMN;Hyd Pdt
Anaerobic Biodeg Prim:		Days	Weeks	Months	Months	
Hydrolysis (t1/2 at pH 7,25C) A:	1	<= Minutes	Hours	Days	>= Months	C-Cl
Hydrolysis (t1/2 at pH 7,25C) B:		Minutes	Hours	Days	Months	
Sorption to Soils/Sediments:	;4	V. Strong	Strong	Moderate	Low	PMN;Hyd Pdt
Migration to Ground Water:	1;1	Negligible	Slow	Moderate	Rapid	PMN;Hyd Pdt
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	

Removal in WWT/POTW (Overall): 99;95 PMN;Hyd Pdt

Bio Comments: Fate Study Summaries are available.
Hyd Pdt Fish log BAF 0 03 (0 9)

Fate Comments: OECD 111 (Hydrolysis) hydrolysis occurred rapidly (pH 4,7,9) @ 50C; OECD 111 (Hydrolysis): t1/2 (pH 4,7,9) 1h/ 1h/ 1h @ 15 0C; OECD 301B (Mod Sturm CO2 ev): 89.3%/28d, RB.

Comments/Telephone Log

Attachments	Update/Upload Time	Update/Upload By
P 22 0162 OECD 121 Adsorption.docx	08/25/2022 10 55	Thomas Webb
P 22 0162 OECD 117 Partition Coefficient.docx	08/25/2022 10 55	Thomas Webb
P 22 0162 OECD 111 Hydrolysis 2.docx	08/25/2022 10 55	Thomas Webb
P 22 0162 OECD 111 Hydrolysis 1.docx	08/25/2022 10 55	Thomas Webb
P 22 0162 OECD 105 Water Solubility.docx	08/25/2022 10 55	Thomas Webb
P 22 0162 OECD 301B Ready Biodegradation.docx	08/25/2022 10 55	Thomas Webb

Attachments	Update/Upload Time	Update/Upload By
P-22-0162 Hyd Pdt.doc	08/25/2022 10:55	Thomas Webb
P-22-0162 Hyd Pdt.xls	08/25/2022 10:55	Thomas Webb

Historic Documents

Attachments	Version Number	Updated/Uploaded Time	Updated/Uploaded By

Current Version Comments

Comment	Update/Upload Time	Update/Upload By