Chemistry Report for Case # P-17-0195

General

Submitter: ███████████	
Contact: ████████	**Contact Telephone No.:** ██████████
TS No.: KD07CQ	
Chemist: Roberts, Justin	**Contractor Support:** Y
PV Init (kg/yr): ████████	**PV Max (kg/yr):** ████████
Binding Option: ☐	**Exposure-Based Review:** ■
Manufacture: ☐	**Import:** ☑

CAS Number: ███████

Chemical Name ██████████
████████████████

Trade Name: ██████

IES Order: 402066

Generic Name: 1,3-Propanediol,2-methylene-, substituted

Chemical Structure

██████████████████
██████████████████
██████████████████
██████████████████

Physical Chemical Properties

Molecular Formula: ██████ ██	**Molecular Weight:** ██████
% < 500:	**% < 1000:**
MP:	**MP Estimate:**

BP: **BP Pressure:**5.00

BP Estimate:<mark>217</mark>

VP (Torr):   **VP Estimate (Torr):**0.14

Water Solubility (g/L):   **Water Soluble Estimate (g/L):**13.6

Log P: **Log P Estimate:**1.31

Physical State — Neat: Liquid   **Physical State — Manuf:**NK -
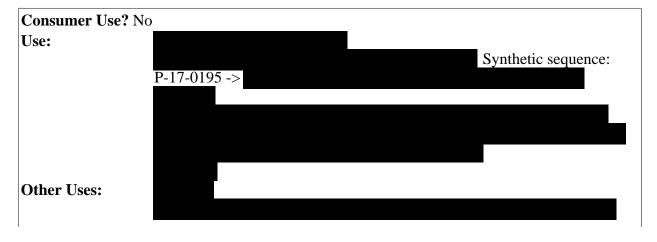   Imported

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Physical State — Processing: NA
Physical State — End Use: Destroyed

Additional Chemical Info

Submitted
data: liquid; BP = ▮▮▮▮ °C at 22.5 torr and 83 °C at 5 torr;
practically insoluble in water; flash point = ▮ °C (Cleveland open cup);
miscible with many organic solvents; solubility in DMSO > 100 g per 100
ml at 25 °C; density = ▮▮ g/cc; refractive index = 1.437 at 25 °C. IR
and 1H NMR spectra were provided. Literature data (STN eprop): BP = ▮ °C
at 70 torr, ▮ °C at 12 torr, and ▮▮ °C at 1 torr; density = ▮▮ at
25 °C. NOMO5 (Class 3) estimated data: from BP = ▮ °C at 22.5 torr: BP =
▮ °C and VP = 0.09 torr; from BP = ▮ °C at 5 torr: BP = ▮ °C and VP
= 0.14 torr. EPI estimated data (input MP = 20 °C), SMILES:
▮▮▮▮▮▮▮▮▮ BP = ▮ °C; VP = 0.976 torr; WS = 13.6 g/L; log P
= 1.31. ACD Labs estimated data (STN pprop): BP = ▮ °C; VP = 0.0871
torr; WS = 19 g/L; log P = 0.977.

Uses

Consumer Use? No
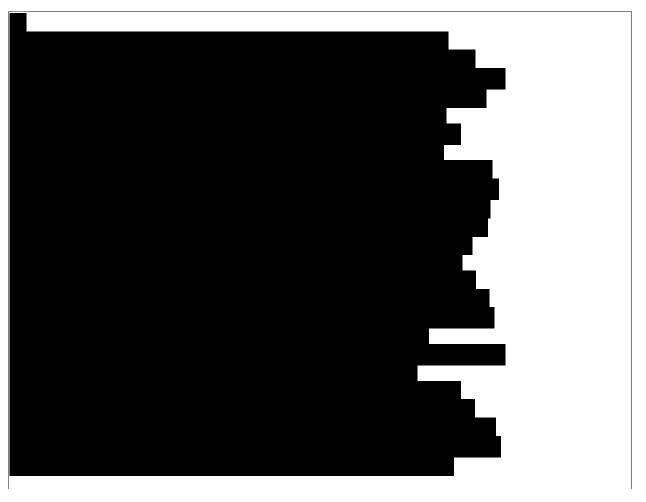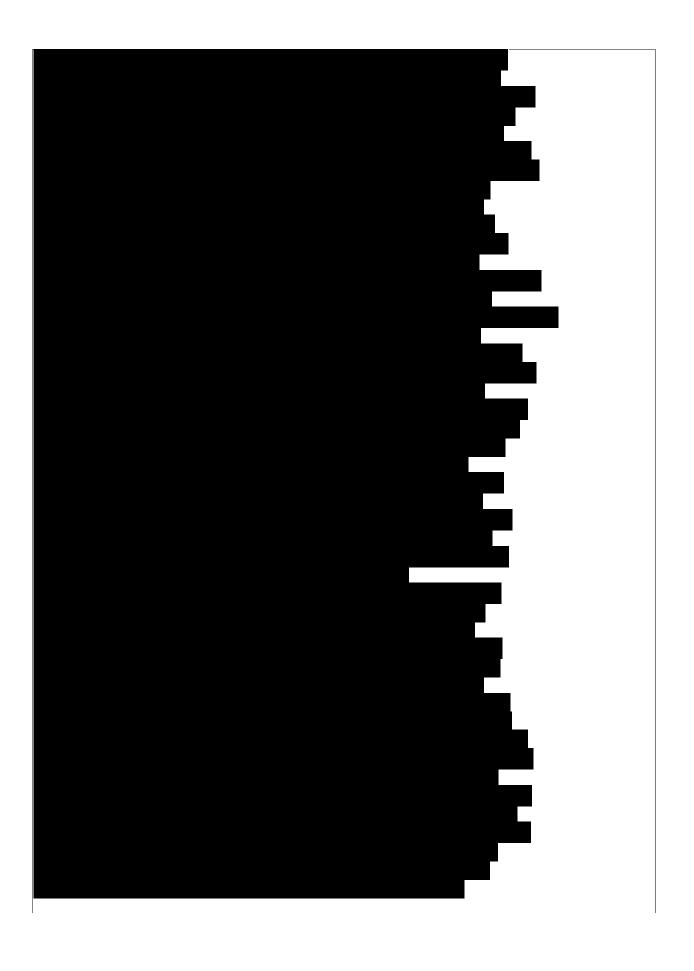**Use:** ▮▮▮▮▮▮▮▮▮▮
                                           Synthetic sequence:
         P-17-0195 -> ▮▮▮▮▮▮▮▮
▮▮▮▮▮▮▮▮▮▮▮▮
▮▮▮▮▮▮▮▮▮▮

Other Uses: ▮▮▮▮▮▮▮▮▮▮

Reaction Description

Pollution Prevention Analysis(P2 Analysis:)

[REDACTED]

Analogs

Analogs:
[REDACTED]

Comments/Telephone Log

Artifact	Update/Upload Time
[REDACTED]	[REDACTED]