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UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

SEP 27 1993

OFFICE OF
PREVENTION, PESTICIDES AND
TOXIC SUBSTANCES

MEMORANDUM

SUBJECT: Reregistration of Picloram Acid TCAI, Triisopropanol Amine (TIPA) Salt, Potassium Salt, and Isooctyl Ester (IOE). List A Chemical Nos. 005101, 005102, 005104, and 005103; Case No. 0096. DowElanco: Response to The Picloram, Salts and Ester Product Chemistry Data Requirements. (MPID Nos. 428408-01 to 428408-11; CBRS # 12289; DP BARCODE: D193574)

FROM: Freshteh Toghrol, Ph.D., Chemist *F. Toghrol*
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Chemistry Branch II: Reregistration Support
Health Effects Division (H7509C)

THRU: William J. Hazel, Ph.D., Section Head *W.J. Hazel*
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TO: Lois Rossi/W. Waldrop, PM 71
Reregistration Branch
Special Review and Reregistration Division (H7508W)

DowElanco has submitted product chemistry (63 series) data (424808-01 to 424808-11) for the Picloram acid 72% T/MP (EPA Reg No. 62719-179), triisopropanol amine (TIPA TGAI) to support picloram TIPA products (EPA Reg. Nos 62719-5, 62719-31, and 62710-182), isooctyl ester (IOE TGAI) to support picloram IOE (EPA Reg. No. 62719-57), and potassium (K-salt) FI 34.7% (EPA Reg. No. 62719-30). These physical chemical characteristics are summarized in Tables 1 through 4 each followed by CBRS conclusions.

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Table 1. Physical and chemical properties of the Picloram potassium salt. Lot No. AGR275251, containing 99.2% picloram K in solid form (MRID No. 428408-01 for all except 63-10), was used to support reregistration of the Picloram potassium salt FI 34.7% (EPA Reg. No. 62719-30).

Guidelines Reference No., 40 CFR §158.190; Name of Property	Description [Method]
63-2. Color	White; [visual]
63-3. Physical state	Solid at 21.8 °C; [visual]
63-4. Odor	No significant odor [smelling]
63-5. Boiling Point	N/A; TGAI is a solid
63-6. Melting Point	Greater than 250 °C [OECD GLN 102 May 19J1; Meltemp melting point apparatus and thermometer]
63-7. Density, bulk density, or specific gravity	Average Relative Density 1.859 at 20 °C [OECD GLN 109 May 1981; analytical balance and volumetric flask]
63-10. Dissociation Constant	$pK_a = 2.2$ [Pulse Polarography] (MRID 428408-09)
63-12. pH	9.18 (for 9.96% solution in water) [ASTM D2110-64; pH meter]
63-13. Stability	Stable at 0, 25, and 50 °C and to mild steel, 304 stainless steel, 316 stainless steel, brass, $MgCl_2 \cdot 6H_2O$, and $FeCl_3 \cdot 6H_2O$ at 50 °C for 28 days [HPLC; K salt was converted to acid and analyzed against standard acid] (HPLC % of theoretical ranged from 100.8 to 103.9;]. The half life in dilute solution in the presence of sunlight was 2.6 days at 25 °C in sterile pH 7 water (data were provided in 1986; MRID 00164943).

CBRS Conclusions Regarding the Picloram Potassium Salt:

The data gaps for picloram potassium salt TGAI regarding color (GLN No. 63-2), physical state (GLN NO. 63-3), odor (GLN No. 63-4), boiling point (GLN No. 63-5), melting point (GLN NO. 63-6), density, bulk density, or specific gravity (GLN No. 63-7),

dissociation constant (GLN No. 63-10), pH (GLN No. 63-12), and stability (GLN No. 63-13) are resolved.

Table 2. Physical and chemical properties of the Picloram Triisopropanolamine salt (TIPA TGAI). Lot No. AGR275680, with 96.8% purity in solid form was used to support reregistration of picloram TIPA salts (EPA Reg. No. 62719-5, 62719-31, and 62719-182; MRID No. 428408-03 for all except 63-10)

Guidelines Reference No., 40 CFR §158.190; Name of Property	Description [Method]
63-2. Color	Light brown/tan; [visual]
63-3. Physical state	Solid at 23.5 °C; [visual]
63-4. Odor	Alcohol like [smelling]
63-5. Boiling Point	N/A; TGAI is a solid
63-6. Melting Point	99-104 °C [OECD GLN 102 May 1981; Meltemp melting point apparatus and thermometer]
63-7. Density, bulk density, or specific gravity	Average Relative Density 1.379 at 20 °C [OECD GLN 109 May 1981; analytical balance and volumetric flask]
63-10. Dissociation Constant	pK _a =2.0 [Normal Pulse Polarography] (MRID 428408-09)
63-12. pH	5.42 (for 9.96% solution in water) [ASTM D2110-64; pH meter]
63-13. Stability	Stable at 0, 25, and 50 °C and to mild steel, 304 stainless steel, 316 stainless steel brass, MgCl ₂ ·6H ₂ O, and FeCl ₃ ·6H ₂ O at 50 °C for 28 days [[HPLC; the picloram salt samples were converted to acid and analyzed against standard acid. HPLC assay % of theoretical ranged from 95.4 to 101.9]. The half life in dilute solution in the presence of sunlight was 2.6 days at 25 °C in sterile pH 7 water (data were provided from 1986; MRID 00164943)

CBRS Conclusions Regarding the Picloram Triisopropanolamine Salt (TIPA TGAI):

The data gaps for the picloram TIPA TGAI regarding color (GLN No. 63-2), physical state (GLN No. 63-3), odor (GLN No. 63-4), boiling point (GLN No. 63-5), melting point (GLN No. 63-6), density, bulk density, or specific gravity (GLN No. 63-7), dissociation constant (GLN No. 63-10), pH (GLN No. 63-12), and stability (GLN No. 63-13) are resolved.

Table 3. Physical and chemical properties of the Picloram acid 72% T/MP (EPA Reg. No. 62719-179). Lot AGR221371 was used to support reregistration of picloram acid 72% T/MP (EPA Reg. No. 62719-179; MRID 428408-02 for all except 63-10 and 63-20).

Guidelines Reference No., 40 CFR §158.190; Name of Property	Description [Method]
63-10. Dissociation Constant	pk _a = 2.3 [Normal Pulse polarography] (MRID 428408-09)
63-14 Oxidizing/Reducing Action	No notable temperature change in the presence of zinc powder, ammonium phosphate, and potassium permanganate dispersed in water [ASTM E680-84]
63-15 Flammability	N/A for solid MPs
63-16 Explodability	No positive result observed at 20.25 inches [Method not given]
63-18 Viscosity	N/A for solid MPs
63-19 Miscibility	N/A for solid MPs
63-20. Corrosion Characteristics	Noncorrosive to epoxy-modified-phenolic Resin Coated with Steel at 122 °F for 33 days [observation of the lining and weight measurement] (428408-02)

CBRS Conclusions Regarding the Picloram Acid T/MP:

The data gaps for the picloram Acid T/MP (EPA Reg. No. 62719-179) regarding dissociation constant (GLN No. 63-10), oxidizing/reducing action (GLN No. 63-14), flammability (GLN No. 63-15), explodability (GLN No. 63-16), viscosity (GLN No. 63-18), miscibility (GLN No. 63-19), and corrosion Characteristics (GLN No. 63-20) are resolved.

Table 4. Physical and chemical properties of the Picloram isooctyl (i.e., 2-ethylhexyl) ester (IOE TGAI). Lot AGR289180, with 89.7% purity in solid form was used to support reregistration of picloram isooctyl ester (EPA Reg. No. 62719-57)

Guidelines Reference No., 40 CFR §158.190;		Description [Method] (Lot No, Purity; MRID No.)																						
Name of Property																								
63-2.	Color	Brown; [visual] (MRID 42840804)																						
63-3.	Physical state	Solid at 19.6 °C [visual] (MRID No. 42840804)																						
63-4.	Odor	phenol like [smelling] (MRID No. 42840804)																						
63-5.	Boiling Point	N/A; TGAI is a solid																						
63-6.	Melting Point	70.2-72.3 °C [OECD GLN 102 May 1981] (MRID No. 42840804)																						
63-7.	Density	Average Relative Density 1.242 at 20 °C [OECD GLN 109 May 1981; analytical balance and volumetric flask] (MRID No. 42840804)																						
63-8.	Solubility	<p>Solvents: solubility (at 25 °C)</p> <p>Water 0.23 ± 0.03 ppm</p> <table border="1"> <thead> <tr> <th>Organic Solvent (at 20 °C)</th> <th>Solubility (g/100 ml)</th> </tr> </thead> <tbody> <tr> <td>Acetone</td> <td>61.9</td> </tr> <tr> <td>ethyl acetate</td> <td>53.9</td> </tr> <tr> <td>methylene chloride</td> <td>77.6</td> </tr> <tr> <td>THF</td> <td>62.4</td> </tr> <tr> <td>Xylene</td> <td>50.4</td> </tr> <tr> <td>Toluene</td> <td>56.5</td> </tr> <tr> <td>Acetonitrile</td> <td>26.6</td> </tr> <tr> <td>2-Propanol</td> <td>13.5</td> </tr> <tr> <td>1-Octanol</td> <td>14.8</td> </tr> <tr> <td>Hexane</td> <td>0.60</td> </tr> </tbody> </table> <p>[Generator column for water solubility, purity not reported; MRID No. 428408-08; GC for organic solvent] (Lot No. AGR74498, with 99.5% purity; MRID No. 428408-10)</p>	Organic Solvent (at 20 °C)	Solubility (g/100 ml)	Acetone	61.9	ethyl acetate	53.9	methylene chloride	77.6	THF	62.4	Xylene	50.4	Toluene	56.5	Acetonitrile	26.6	2-Propanol	13.5	1-Octanol	14.8	Hexane	0.60
Organic Solvent (at 20 °C)	Solubility (g/100 ml)																							
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1-Octanol	14.8																							
Hexane	0.60																							

Guidelines Reference No., 40
CFR §158.190;

Name of Property	Description [Method] (Lot No, Purity; MRID No.)
63-9. Vapor Pressure	7 X 10 ³ at 25 °C Extrapolated from ten measurements in the temperature range of 55.0 to 69.1 °C using the Knudsen-effusion weight loss method. Dow Report ML-AL 84-40252 1984] (Lot No AGR 074498, with 98.4% purity; MRID 248408-06)
63-10 Dissociation Constant	Dissociation constant is not feasible because the ester will hydrolyze during the process of determining the dissociation constant
63-11 Octanol/Water Partition Coefficient	Log ₁₀ K _{ow} = 5.90 ± 0.06 at 25 °C [Generator column method] (Lot No AGR074498, with 98.4% purity; MRID 428408-07)
63-12. pH	N/A; Picloram isooctyl ester is not dispersable in water, it is a waxy low melting solid. (MRID No. 428408-04)
63-13 Stability	Stable to mild steel, 304 stainless steel, 316 stainless steel, brass, MgCl ₂ .6H ₂ O, and FeCl ₃ .6H ₂ O at 0, 25, and 50 °C for 28 days [HPLC; the picloram salt samples were converted to acid and analyzed against standard acid; % ai of theoretical ranged from 90.9 to 102.5; MRID No. 428408-04). The half life in dilute solution in the presence of sunlight was 2.6 days at 25 °C in sterile pH 7 water (data were provided from 1986; MRID 00164943)

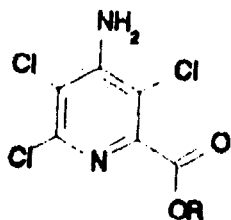
DowElanco also indicates that the preliminary analysis data of five batches of the picloram IOE will be provided later. However, they do submit one analysis of a laboratory scale batch of picloram IOE which has been submitted for toxicological studies (MRID 428408-11).

CBRS Conclusions Regarding the Picloram Isooctyl Ester (IOE TGAI):

The data gaps for the picloram isooctyl ester (IOE TGAI) regarding color (GLN No. 63-2), physical state (GLN NO. 63-3), odor (GLN No. 63-4), melting point (GLN NO. 63-6), density, bulk density, or specific gravity (GLN No. 63-7), solubility (GLN NO. 63-8, vapor pressure (GLN No. 63-9), dissociation constant (GLN NO. 63-10), octanol/water partition coefficient (GLN No. 63-11), pH (GLN No. 63-12), and stability (GLN No. 63-13) are resolved.

CBRS awaits the preliminary preliminary analysis data of five batches of the picloram IOE and will review those data upon receipt.

PICLORAM (TRIISOPROPANOL AMINE, ISOCTYL ESTER, AND POTASSIUM SALT)



- R = NH(CH₂CH(OH)CH₃); Shaughnessy No. 005102.
- R = C₈H₁₇; Shaughnessy No. 005103
- R = H; Shaughnessy No. 005101.
- R = K; Shaughnessy No. 005104.

cc: Picloram S.F., R.F., F. Toghrol, Reg. Std. File, Circ.
 RDI: W. Hazel (9/20/93); M. Metzger (9/21/93); E. Zager (9/23/93)
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