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**OPP OFFICIAL RECORD  
HEALTH EFFECTS DIVISION  
SCIENTIFIC DATA REVIEWS  
EPA SERIES 361**

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

OFFICE OF  
PREVENTION, PESTICIDES  
AND TOXIC SUBSTANCES

**MEMORANDUM**

Date: 24-JUN-2005

Subject: Flumiclorac Pentyl Tolerance Reassessment Eligibility Decision (TRED). Product Chemistry Considerations.

DP Barcode: D302003

PC Code: 128724

From: William H. Donovan, Ph.D., Chemist *William H. Donovan*  
Reregistration Branch 3 (RRB3)  
Health Effects Division (HED) (7509C)

Through: Danette Drew, Branch Senior Scientist *DD*  
RRB3, HED (7509C)

To: Twanda Spears, CRM  
Reregistration Branch III  
Special Review and Reregistration Division (SRRD) (7508C)

This document was originally prepared under contract by Dynamac Corporation (20440 Century Boulevard, Suite 100; Germantown, MD 20874; submitted 01/26/2005). The document has been reviewed by the HED and revised to reflect current OPP policies.

JUN 28 2005

Flumiclorac Pentyl

TRED: Product Chemistry Considerations

Barcode: D302003

**Executive Summary**

Flumiclorac pentyl [(2-chloro-4-fluoro-5-(1,3,4,5,6,7-hexahydro-1,3-dioxo-2H-isoindol-2-yl)phenoxy)acetic acid, pentyl ester] is an N-phenylphthalimide derivative herbicide used for the control of broadleaf weeds. Its mode of action is through the accumulation of porphyrins in susceptible plants; the photosensitizing action of accumulated porphyrins may cause membrane lipid peroxidation which leads to irreversible damage of membrane function and structure in the plant. Flumiclorac pentyl is registered for postemergence application to field corn and soybeans; registration for use on cotton as a defoliant is pending.

Flumiclorac pentyl is not a reregistration list chemical; no comprehensive review document has been issued to date. Data were initially submitted in conjunction with an experimental-use petition for flumiclorac pentyl on field corn and soybeans (PP#2G4078; D174474, 7/28/92, J. Garbus). Additional product chemistry data have been reviewed by the Registration Division (RD).

Additional product chemistry data are required for the only registered manufacturing-use product, the Valent 98.6% T (EPA Reg. No. 59639-81), concerning UV/visible absorption. Provided that the registrant submits the data required in the attached data summary table for the flumiclorac pentyl T/TGAI, and either certifies that the suppliers of beginning materials and the manufacturing process for the flumiclorac pentyl T/TGAI have not changed or submits a complete updated product chemistry data package, HED has no objections to renewing the registration of flumiclorac pentyl as required under FQPA with respect to product chemistry data requirements.

**Product Chemistry Deficiencies**

Additional data are required concerning UV/visible absorption (OPPTS 830.7050) for the Valent U.S.A. Corporation 98.6% T (EPA Reg. No. 59639-81).

**Background****Identification of Active Ingredient**

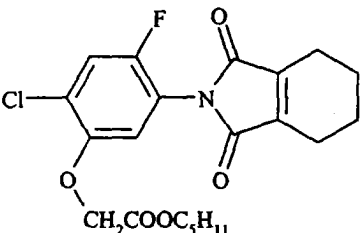
The PC code and nomenclature of flumiclorac pentyl are listed below in Table 1. The physicochemical properties of flumiclorac pentyl are listed in Table 2.

Flumiclorac Pentyl

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**TABLE 1. Flumiclorac Pentyl Nomenclature**

Chemical Structure	
Common name	Flumiclorac pentyl
Company experimental name	S-23031 or V-23031
Molecular Formula	C <sub>21</sub> H <sub>23</sub> ClFNO <sub>5</sub>
Molecular Weight	423.9
IUPAC name	Pentyl (2-chloro-5 (cyclohex-1-ene-1,2-dicarboximido)-4-fluorophenoxy) acetate
CAS name	Pentyl[2-chloro-4-fluoro-5-(1,3,4,5,6,7- hexahydro-1,3-dioxo-2H-isoindol-2-yl)phenoxy]acetate
CAS #	87546-18-7
PC Code	128724

**TABLE 2. Physicochemical Properties of Flumiclorac Pentyl**

Parameter	Value	Reference
Melting point	88.9-90.1 °C	PP#2G4078; D174474, 7/28/92, J. Garbus
pH	6.03 at 25 °C	
Density, bulk density, or specific gravity	1.3316 g/mL at 20 °C	
Water solubility	0.189 mg/L at 25 °C	
Solvent solubility	<u>g/100 mL at 25 °C:</u> hexane 0.328 n-octanol 1.60 methanol 4.78 Solvesso 150 27.1 acetonitrile 58.9 acetone 59.0 tetrahydrofuran 69.7 N-methyl 2-pyrrolidinone 134.0 methylene chloride 288.0	
Vapor pressure	<1 x 10 <sup>-7</sup> mm Hg at 22.4 °C	
Dissociation constant, pK <sub>a</sub>	No dissociation at pH ≤7; flumiclorac pentyl decomposes at pH ≥9.	
Octanol/water partition coefficient	Log P <sub>ow</sub> = 4.99 at 19.7-21.0 °C	
UV/visible absorption spectrum	Not available	

### Manufacturing-use Products

A search of the OPPIN product listings conducted 12/04 identified a single manufacturing-use product (MP) registered under PC Code 128724: the Valent U.S.A. Corporation 98.6% T (EPA

Flumiclorac Pentyl

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Reg. No. 59639-81).

**830.1550-7950 Product Chemistry Data Requirements**

The current status of the product chemistry data requirements for the flumiclorac pentyl T/TGAI is presented in the attached data summary table. Refer to this table for a listing of the outstanding product chemistry data requirements.

Flumiclorac Pentyl

TRED: Product Chemistry Considerations

Barcode: D302003

Case No. Not applicable

Chemical No. 128724

Case Name: Flumiclorac pentyl

Registrant: Valent U.S.A. Corporation

Product(s): 98.6% T (EPA Reg. No. 59639-81)

**PRODUCT CHEMISTRY DATA SUMMARY**

Guideline Number	Requirement	Are Data Requirements Fulfilled? <sup>1</sup>	MRID Number <sup>2</sup>
830.1550	<b>Product identity and composition</b>	Y	<b>42187401, 42825801</b> <sup>3</sup> , CSF 3/9/95 <sup>4</sup>
830.1600	Description of materials used to produce the product	Y	42187401, 42825801 <sup>3</sup>
830.1620	Description of production process	Y	42187401, 42825801 <sup>3</sup>
830.1670	Discussion of formation of impurities	Y	42187401, 42825801 <sup>3</sup>
830.1700	Preliminary analysis	Y	42187403, 42825802 <sup>3</sup> , 43552301 <sup>4</sup>
830.1750	Certified limits	Y	42187401, 42187403, CSF 3/9/95 <sup>4</sup>
830.1800	<b>Enforcement analytical method</b>	Y	<b>42187403, 43552302</b> <sup>4</sup>
830.6302	Color	Y	42187405, 43552303 <sup>4</sup>
830.6303	Physical state	Y	42187405
830.6304	Odor	Y	42187405
830.6313	Stability to normal and elevated temperatures, metals, and metal ions	Y	42187405
830.6314	Oxidation/reduction: chemical incompatibility	Y	42825803 <sup>3</sup>
830.6315	Flammability	N/A <sup>5</sup>	
830.6316	Explosibility	Y	42187405
830.6317	Storage stability	Y	42187405
830.6319	Miscibility	N/A <sup>5</sup>	
830.6320	Corrosion characteristics	Y	42187405
830.7000	pH	Y	42187405
830.7050	UV/Visible absorption	N	
830.7100	Viscosity	N/A <sup>5</sup>	
830.7200	Melting point/melting range	Y	42187405
830.7220	Boiling point/boiling range	N/A <sup>5</sup>	
830.7300	Density/relative density/bulk density	Y	42187405
830.7370	Dissociation constants in water	Y	42187405
830.7550	Partition coefficient (n-octanol/water), shake flask method	Y	42187405
830.7840	Water solubility: column elution method; shake flask method	Y	42187405
830.xxxx	Solvent solubility	Y	42187405
830.7950	Vapor pressure	Y	42187405

<sup>1</sup> Y = Yes; N = No; N/A = Not Applicable.<sup>2</sup> **Bolded** references were reviewed under PP#2G4078, D174474, 7/28/92, J. Garbus, and all other references were reviewed as noted.<sup>3</sup> RD Memorandum, D195818, 3/22/94, S. Mathur.<sup>4</sup> RD Memorandum, D216031, 6/15/95, A. Smith.<sup>5</sup> Data are not required because the T/TGAI is a solid at room temperature.

**BIBLIOGRAPHY****Study Citations**

42187401 Takemoto, I. (1991) Product Identity and Disclosure of Ingredients: Description of Beginning Materials and Manufacturing Process: Description of Formation of Impurities for Technical S-23031: Lab Project Number: 91-031-06. Unpublished study prepared by Sumitomo Chemical Co., Ltd. 44 p.

42187403 Furuta, R. (1991) Preliminary Analysis of Product Samples: Certification of Ingredient Limits: Analytical Method to Verify Certified Limits of S-23021 Technical: Lab Project Number: 91-031-09. Unpublished study prepared by Sumitomo Chemical Co., Ltd. 68 p.

42187405 Pesselman, R.; Yamada, H.; Sweetapple, G.; et al. (1991) Physical and Chemical Characteristics of V-23031 Technical: Lab Project Number: 91-031-02. Unpublished study prepared by Ricerca, Inc., Sumitomo Chemical Co., Ltd., and Hazleton Labs. 335 p

42825801 Takemoto, I.; Tsuda, S. (1991) V-23031 Technical: Product Chemistry: Supplemental: Lab Project Number: 93-RES-008. Unpublished study prepared by Sumitomo Chemical Co., Ltd. 83 p.

42825802 Furuta, R. (1993) V-23031 Technical: Product Chemistry: Supplemental: Lab Project Number: 93-RES-001. Unpublished study prepared by Sumitomo Chemical Co., Ltd. 4 p.

42825803 Radcliffe, M. (1993) V-23031 Technical: Product Chemistry: Supplemental: Lab Project Number: 93-RES-002. Unpublished study prepared by Valent USA Corp. 4 p.

43552301 Okumura, T. (1994) Preliminary Analysis of Product Samples of Flumiclorac Pentyl Technical (S-23031): Lab Project Number: 310601: SAP-40-0023. Unpublished study prepared by Sumitomo Chemical Co., Ltd. 20 p.

43552302 Okumura, T. (1994) Analytical Method to Verify Certified Limits of Flumiclorac Pentyl Technical (S-23031): Lab Project Number: SAA-40-0045. Unpublished study prepared by Sumitomo Chemical Co., Ltd. 14 p.

43552303 Okumura, T. (1994) Color Determination of Flumiclorac Pentyl Technical (S-23031): Lab Project Number: 310602: SAP-40-0025. Unpublished study prepared by Sumitomo Chemical Co., Ltd. 9 p.

Flumiclorac Pentyl

TRED: Product Chemistry Considerations

Barcode: D302003

**Agency Memoranda Citations**

DP Barcode(s): D174474  
Subject: PP#2G4078: New Chemical EUP: V-23031, Flumiclorac-Pentyl on Field Corn and Soybeans. Evaluation of Analytical Methods and of Residue Data.  
From: J. Garbus  
To: J. Miller/D. Kenny and A. Kocialski  
Dated: 7/28/92  
MRID(s): 42187400-42187405, 42169849-42169859, and 42187407-42187408.

DP Barcode(s): RD D195818  
Subject: Product Chemistry Review on Series 61 and Series 62 (supplemental data) for the Chemical Flumiclorac (Tech.). Waiver Request for 63-14.  
From: S. Mathur  
To: J. Miller  
Dated: 3/22/94  
MRID(s): 42825801-42825803

DP Barcode(s): RD D216031  
Subject: Product Chemistry Review of Flumiclorac Pentyl Technical (S-23031).  
From: A. Smith  
To: D. Kenny  
Dated: 6/15/95  
MRID(s): 43552301-43552303



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<b>Chemical:</b>	<b>Flumiclorac</b>
<b>PC Code:</b>	<b>128724</b>
<b>HED File Code</b>	<b>11000 Chemistry Reviews</b>
<b>Memo Date:</b>	<b>06/24/2005</b>
<b>File ID:</b>	<b>DPD302003</b>
<b>Accession Number:</b>	<b>412-05-0098</b>

**HED Records Reference Center**  
**07/11/2005**