

US EPA ARCHIVE DOCUMENT



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

OFFICE OF  
PREVENTION, PESTICIDES AND  
TOXIC SUBSTANCES

April 21, 2005

**ACTION MEMORANDUM**

**SUBJECT:** Inert Ingredient Tolerance Reassessment - Diethylene Glycol Abietate

**FROM:** Dan Rosenblatt, Chief  
Minor Use, Inerts, and Emergency Response Branch

**TO:** Lois A. Rossi, Director  
Registration Division

**I. FQPA REASSESSMENT ACTION**

**Action:** Reassessment of one (1) inert ingredient exemption from the requirement of a tolerance.

**Chemical and Use Summary:** See table below.

Tolerance Exemption Being Reassessed				
Tolerance Exemption Expression	CAS Reg No.	40 CFR §	Use Pattern (Pesticidal)	List Classification
Diethylene glycol abietate	10107-99-0	180.910 <sup>1/</sup>	Surfactant, related adjuvants of surfactants	--

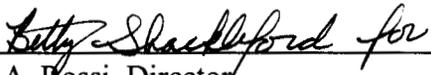
1. Residues listed in 40 CFR §180.910 [formerly 40 CFR§ 180.100(c)] are exempted from the requirement of a tolerance when used as inert ingredients in pesticide formulations when applied to raw agricultural commodities and growing crops.

**List Classification Determination:** Diethylene glycol abietate is uncategorized as to list classification status. Based upon the reasonable certainty of no harm safety finding, diethylene glycol abietate can be classified as a List 4B inert ingredient.

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**II. MANAGEMENT CONCURRENCE**

I concur with the reassessment of the one (1) exemption from the requirement of a tolerance for the inert ingredient, diethylene glycol abietate and with the List classification determination, as described above. I consider the one (1) exemption from the requirement of a tolerance for diethylene glycol abietate established in 40 CFR §180.910 [formerly 40 CFR§180.1001(c)] to be maintained and reassessed as of the date of my signature, below. A Federal Register Notice regarding this tolerance exemption reassessment decision will be published in the near future.

  
\_\_\_\_\_  
Lois A. Rossi, Director  
Registration Division

Date: 4/27/05

cc: Debbie Edwards, SRRD  
Joe Nevola, SRRD

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April 21, 2005

**MEMORANDUM**

SUBJECT: Reassessment of the Exemption from the Requirement of a Tolerance for Diethylene Glycol Abietate

FROM: Kerry Leifer, Inerts Team Leader  
Minor Use, Inerts and Emergency Response Branch  
Registration Division (7505C)

Handwritten signature of Kerry Leifer in black ink.

THRU: Pauline Wagner, Inerts Coordinator  
Registration Division (7505C)

Handwritten signature of Pauline Wagner in black ink, dated 4/21/05.

TO: Dan Rosenblatt, Chief  
Minor Use, Inerts and Emergency Response Branch  
Registration Division (7505C)

**Background**

Attached is the science assessment for diethylene glycol abietate. This assessment summarizes available information on the use, physical/chemical properties, toxicological effects, exposure profile, and environmental fate and ecotoxicity of diethylene glycol abietate. The purpose of this document is to reassess the existing exemption from the requirement of a tolerance for residues of diethylene glycol abietate as required under the Food Quality Protection Act (FQPA).

**Executive Summary**

This report evaluates diethylene glycol abietate, a pesticide inert ingredient for which an exemption from the requirement of a tolerance exists for its residues when used in pesticide

formulations applied to growing crops only under 40 CFR §180.910 for use as a surfactant and related adjuvant of a surfactant.

There are no readily available toxicity data on diethylene glycol abietate. However, toxicity data do exist for various rosin alcohol and polyol esters, including glycerol esters of rosin, an analog of ethylene glycol abietate. The Joint WHO/FAO Expert Committee on Food Additives (JECFA) has considered data on the toxicity and bioavailability of glycerol esters of wood rosin and has concluded that glycerol esters of wood rosin are nonbioavailable, with no adverse effects identified at limit dose levels of 2500 mg/kg/day in a subchronic oral toxicity study in rats. A structure activity relationship analysis of diethylene glycol abietate was conducted by the Office of Pollution Prevention and Toxics (OPPT) Structure Activity Team. The OPPT assessment concluded that diethylene glycol abietate is poorly absorbed via all routes of exposure and is of low-moderate concern for human health effects, with the only identified health concerns being dermal and respiratory sensitization.

There are no available aquatic toxicity studies on diethylene glycol abietate; the OPPT Structure Activity Team rated diethylene glycol abietate as high concern for chronic toxicity to fish, algae, and aquatic invertebrates. Based on the environmental fate characteristics of diethylene glycol abietate, coupled with its use patterns as a pesticide inert ingredient, it is unlikely that the pesticide inert ingredient use of diethylene glycol abietate would result in water concentrations above the 1 ppb level of concern for chronic toxicity to nontarget aquatic organisms.

Taking into consideration all available information on diethylene glycol abietate, it has been determined that there is a reasonable certainty that no harm to any population subgroup will result from aggregate exposure to diethylene glycol abietate when considering dietary exposure and all other non-occupational sources of pesticide exposure for which there is reliable information. Therefore, it is recommended that the exemption from the requirement of a tolerance established for residues of diethylene glycol abietate in/on raw agricultural commodities can be considered reassessed as safe under section 408(q) of the FFDCA.

## **I. Introduction**

This report evaluates diethylene glycol abietate (CAS Reg. No. 10107-99-0), a pesticide inert ingredient for which an exemption from the requirement of a tolerance exists for its residues when used in pesticide formulations applied to growing crops only under 40 CFR §180.910 [formerly 40 CFR §180.1001(c)].

Diethylene glycol abietate is an ester of diethylene glycol and abietic acid, a carboxylic acid that is found in rosin, a naturally-occurring solid resin derived primarily from coniferous plants. Alcohol and polyol esters of rosin are used as tackifying agents in pressure sensitive adhesives and, as in the case of rosin glycerol ester, as a direct food additive in chewing gum bases and citrus beverages.

## II. Use Information

### Pesticides

The tolerance exemption for the inert ingredient diethylene glycol abietate is given in Table 1 below.

<b>Table 1. Tolerance Exemption Being Reassessed in this Document</b>				
<b>Tolerance Exemption Expression</b>	<b>CAS Reg No.</b>	<b>40 CFR §</b>	<b>Use Pattern (Pesticidal)</b>	<b>List Classification</b>
Diethylene glycol abietate	10107-99-0	180.910 <sup>1/</sup>	Surfactant, related adjuvants of surfactants	--

1. Residues listed in 40 CFR §180.910 [formerly 40 CFR§ 180.100(c)] are exempted from the requirement of a tolerance when used as inert ingredients in pesticide formulations when applied to growing crops or to raw agricultural commodities after harvest.

### Other Uses

No other uses were identified for diethylene glycol abietate.

## III. Physical and Chemical Properties

Some of the physical and chemical characteristics of diethylene glycol abietate including a chemical structure are found in Appendix A.

## IV. Hazard Assessment

### **A. Hazard Profile**

There are no readily available toxicity data on diethylene glycol abietate (TOXNET 2005). However, toxicity data do exist for various rosin alcohol and polyol esters, including glycerol esters of rosin, an analog of ethylene glycol abietate. The Joint WHO/FAO Expert Committee on Food Additives (JECFA) has considered data on the toxicity and bioavailability of glycerol esters of wood rosin as part of its evaluation of glycerol esters of wood rosin. On the basis of studies confirming nonbioavailability (i.e., glycerol esters of wood rosin are shown to be stable in the human gastrointestinal tract) as well as a 13-week toxicity study in rats in which the

no observed effect level (NOEL) was 2500 mg/kg bw per day, JECFA allocated an ADI<sup>1</sup> of 0-25 mg/kg bw (JECFA 1996).

A structure activity relationship analysis of diethylene glycol abietate was conducted by the Office of Pollution Prevention and Toxics (OPPT) Structure Activity Team. The OPPT assessment concluded that diethylene glycol abietate is expected to be poorly absorbed via all routes of exposure and that diethylene glycol abietate is of a low-moderate concern for human health effects, with a potential concern for dermal and respiratory sensitization based on abietic acid. The OPPT Structure Activity Team assessment report is included in Appendix A.

## **B. Toxicological Data**

No references to toxicity studies on diethylene glycol abietate were identified in the open literature.

## **C. Metabolism And Pharmacokinetics**

The OPPT Structure Activity Team assessment notes that diethylene glycol abietate is poorly absorbed through the gastrointestinal (GI) tract. Studies on absorption, distribution, metabolism, and excretion have shown that essentially the entire amount of ingested glycerol esters of rosin are excreted unchanged in the feces (JECFA 1996).

## **D. Special Considerations for Infants and Children**

Diethylene glycol abietate is of low concern for systemic human health effects, as toxicity data on other rosin esters demonstrate no adverse effects and diethylene glycol abietate itself is poorly absorbed via all routes of exposure. There are no indications that children and infants would be more susceptible to adverse health effects resulting from exposure to diethylene glycol abietate. A safety factor analysis has not been used to assess the risks resulting from the use of diethylene glycol abietate as a pesticide inert ingredient and an additional tenfold safety factor for the protection of infants and children is unnecessary.

## **V. Exposure Assessment**

Diethylene glycol abietate is poorly absorbed via all routes of exposure, therefore no further dermal, oral, or inhalation exposure assessment is necessary.

## **VI. Aggregate Exposures**

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<sup>1</sup> ADI (Acceptable Daily Intake): An estimate by JECFA of the amount of a food additive, expressed on a body weight basis, that can be ingested daily over a lifetime without appreciable health risk

In examining aggregate exposure, FFDC section 408 directs EPA to consider available information concerning exposures from the pesticide residue in food and all other non-occupational exposures, including drinking water from ground water or surface water and exposure through pesticide use in gardens, lawns, or buildings (residential and other indoor uses).

For diethylene glycol abietate, a qualitative assessment for all pathways of human exposure (food, drinking water, and residential) is appropriate given the lack of human health concerns associated with exposure to diethylene glycol abietate.

## **VII. Cumulative Exposure**

Section 408(b)(2)(D)(v) of the FFDC section 408 requires that, when considering whether to establish, modify, or revoke a tolerance, the Agency consider "available information" concerning the cumulative effects of a particular pesticide's residues and "other substances that have a common mechanism of toxicity."

Unlike other pesticides for which EPA has followed a cumulative risk approach based on a common mechanism of toxicity, EPA has not made a common mechanism of toxicity finding as to diethylene glycol abietate and any other substances and this material does not appear to produce a toxic metabolite produced by other substances. For the purposes of this tolerance action, therefore, EPA has not assumed that diethylene glycol abietate has a common mechanism of toxicity with other substances. For information regarding EPA's efforts to determine which chemicals have a common mechanism of toxicity and to evaluate the cumulative effects of such chemicals, see the policy statements released by EPA concerning common mechanism determinations and procedures for cumulating effects from substances found to have a common mechanism on EPA's website at <http://www.epa.gov/pesticides/cumulative/>

## **VIII. Environmental Fate Characterization/Drinking Water Considerations**

The OPPT Structure Activity Team assessment of diethylene glycol abietate noted that it is slightly soluble in water and strongly sorbed to soils and sediments resulting in negligible migration to ground water. Based on these conclusions, diethylene glycol abietate is not expected to be present in drinking water sources as a result of pesticide inert ingredient use. Some estimated environmental fate properties of diethylene glycol abietate are given in Appendix A.

## **IX. Human Health Risk Characterization**

The OPPT Structure Activity Team has identified diethylene glycol abietate as being of low-moderate concern for human health effects, with the only identified concern being a potential concern for dermal and respiratory sensitization based on abietic acid. Dermal sensitization testing is required to support the registration of all pesticide products under the

Federal Insecticide, Fungicide and Rodenticide Act (FIFRA). Any product that is a dermal sensitizer or which tests positive for dermal sensitization must bear the appropriate precautionary labeling statement. Any potential dermal sensitization concerns related to diethylene glycol abietate would be addressed by the requisite dermal sensitization testing and, if necessary, mitigated through the use appropriate precautionary labeling. Residential or nonoccupational exposure to diethylene glycol abietate as a result of its use as a pesticide inert ingredient is negligible, therefore respiratory sensitization is unlikely.

Taking into consideration all available information on diethylene glycol abietate, it has been determined that there is a reasonable certainty that no harm to any population subgroup will result from aggregate exposure to diethylene glycol abietate when considering dietary exposure and all other nonoccupational sources of pesticide exposure for which there is reliable information. Therefore, it is recommended that the exemption from the requirement of a tolerance established for residues of diethylene glycol abietate in/on raw agricultural commodities can be considered reassessed as safe under section 408(q) of the FFDCFA.

#### **X. Ecotoxicity and Ecological Risk Characterization**

There are no available aquatic toxicity studies on diethylene glycol abietate (ECOTOX, 2002). The OPPT Structure Activity Team rated diethylene glycol abietate as high concern for chronic toxicity to fish, algae, and aquatic invertebrates with a concern concentration of 1 ppb (Appendix A). Based on the environmental fate characteristics of diethylene glycol abietate (see unit VIII above), coupled with its use patterns as a pesticide inert ingredient, it is unlikely that the pesticide inert ingredient use of diethylene glycol abietate would result in water concentrations above the level of concern for chronic toxicity to nontarget aquatic organisms.

#### **References:**

ECOTOX 2002. U.S. Environmental Protection Agency. 2002. ECOTOX User Guide: ECOTOXicology Database System. Version 3.0. <http://www.epa.gov/ecotox/>  
Search terms: Diethylene glycol abietate; CAS Reg. No. 10107-99-0 (March 9, 2005)

TOXNET. 2005. Hazardous Substance Data Bank (HSDB). On-line Scientific Search Engine, National Library of Medicine, National Institute of Health. <http://www.toxnet.nlm.nih.gov>.  
Search term: Diethylene glycol abietate; CAS Reg. No. 10107-99-0 (March 9, 2005)

JECFA 1996. Joint WHO/FAO Expert Committee on Food Additives (JECFA). Glycerol Ester of Wood Rosin. Food Additive Series No. 37. World Health Organization. Geneva.  
<http://www.inchem.org/documents/jecfa/jecmono/v37je02.htm>

**APPENDIX A**

**OPPT SAT Review of Diethylene glycol abietate**

<b>STRUCTURE ACTIVITY TEAM REPORT</b>		ver. 04/98	CBI? (YES/NO)
<b>Case #:</b>	Z-05-0005	<b>DCN:</b>	
<b>SAT Date:</b>	12/7/2004	<b>SAT Chair:</b>	L. Keifer
<b>Submitter:</b>			
<b>Chemical Name:</b>			
1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, 2-(2-hydroxyethoxy)ethyl ester, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]-			
<b>CAS RN:</b>	10107-99-0	<b>Trade Name:</b>	
<b>Structure</b>			
<b>Molecular Formula:</b>		C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>	
<b>Molecular Wt.</b>	391	<b>WT%&lt;500:</b>	<b>WT%&lt;1000:</b>
<b>MP:</b>		<b>BP:</b>	452 <b>Eq. Wt:</b>
<b>H2O Sol (g/L):</b>	0.00023	<b>v.p.</b>	<0.000001
<b>Max. Prod. Volume (kg/yr):</b>		<b>Physical State:</b>	Liquid (est)
<b>USE:</b>			
Pesticide Inert:			
<b>Related Case Numbers</b>		<b>Case Role</b>	
<b>Related Case Numbers</b>		<b>Case Role</b>	
<b>Related Case Numbers</b>		<b>Case Role</b>	
<b>Focus</b>	<b>Date:</b>	<b>Results:</b>	

## STRUCTURE ACTIVITY TEAM REPORT

12/08/04

CASE NUMBER: Z05-0005

RELATED CASES:

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN:	HEALTH	ECOTOX
LEVEL OF CONCERN:	1-2	3

KEYWORDS: SENS-L,S  
AQUATOX

SUMMARY OF ASSESSMENT

FATE: Liquid  
 LogKow = 5.50(E); S (mg/L, 25°C) = 1.6(E); H < 1.00E-8(E)  
 MP (C) < 20(ICB); BP (C) > 400(E); VP @ 25C (mm) < 1.0E-6(E)  
 LogKoc = 3.62(E); LogBCF = 3.53(E);  
 POTW removal (%) = 90 via sorption  
 Time for complete ultimate aerobic biodeg ≥ mo  
 PBT Potential: P2B2T1  
 Sorption to soils/sediments = v.strong  
 \*CEB FATE: Migration to ground water = negl

HEALTH: Expect poor absorption via all routes. Concern for dermal and respiratory sensitization based on abietic acid.

\*CEB HEALTH: Low moderate concern

ECOTOX: Predicted toxicity (P) and measured (M) values in mg/L (ppm) are:

fish 96-h LC50	=	*	P
daphnid 48-h LC50	=	*	P
green algal 96-h EC50	=	0.040	P
fish chronic value	=	0.010	P
daphnid ChV	=	0.007	P
algal ChV	=	0.030	P

Predictions are based on SARs for esters; SAR chemical class = ester-triC6cyclic; MW391; log Kow = 6.0 (ClogP), 5.5 (EPI); liquid (P) with mp < 20 C (P); pH7; effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150.0 mg/L as CaCO3; and TOC <2.0 mg/L;

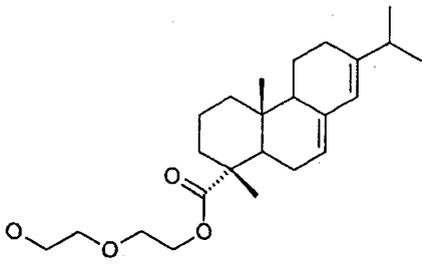
high concern for chronic toxicity only;

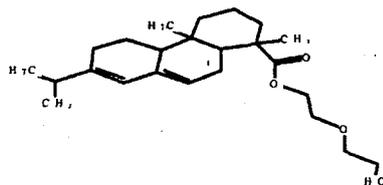
assessment factor = 10.0

concern concentration = 0.001 mg/L (ppm)

\*CEB ECOTOX: All releases to water with CC = 1 ppb

SAT Co-chair: Leonard Keifer 564-8916

NCSAB SAT REPORT			CBI? (Y/N):		
PMN: Z-05-0005		CAS RN: 10107-99-0			
Chemical Name: 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, 2-(2-hydroxyethoxy)ethyl ester, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]-				Analog:	
				Production Volume:	
Structure:					
					
Use:					
Pesticide Inert.					
Formula: C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>			Eq Wt:		
Mol Weight: 390.57		Wt% < 500:		Wt% < 1000	
MP:		BP: 452		VP: < 0.000001	
H <sub>2</sub> O Sol (g/L): 0.230		0.00023		Physical State: Liquid (est) Log P: 6.03 (CLOGP)	
Endpoint (mg/L)	Est. Value	Meas. Value	Comments		
Fish 96-h	*		5.5 (E)		
Daphnid 48-h	*				
Algal 96-h	0.038				
Fish ChV	0.010				
Daphnid ChV	0.007				
Algal ChV	0.032				
BCF					
CHEMICAL CLASS:			SAR: <i>ls/er - <del>tricyclic</del> tri cyclic (G6)</i>		
ECOTOX CONCERN	<input checked="" type="radio"/> H	<input type="radio"/> M	<input type="radio"/> L	CONCERN CONCENTRATION 0.001	
DATE 12/7/04			ASSESSOR:		



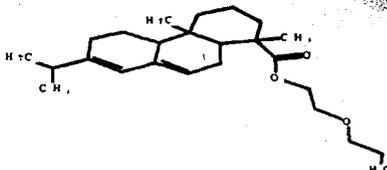
SMILES : OCCOCCOC(=O)C1(C)C2CC=C3C=C(C(C)C)CCC3C2(C)CCC1  
 CHEM :  
 CAS Num:  
 ChemID1:  
 ChemID2:  
 ChemID3:  
 MOL FOR: C24 H38 O4  
 MOL WT : 390.57  
 Log Kow: 6.03 (User entered)  
 Melt Pt: 25.00 deg C  
 Wat Sol: 0.3664 mg/L (calculated)

ECOSAR v0.99g Class(es) Found

-----  
 Esters

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	0.162
Esters	: Fish	96-hr	LC50	0.413 *
Esters	: Daphnid	48-hr	LC50	0.067
Esters	: Green Algae	96-hr	EC50	0.038
Esters	: Green Algae		ChV	0.032
Esters	: Fish		ChV	0.010

Note: \* = asterick designates: Chemical may not be soluble enough to measure this predicted effect.  
 Fish and daphnid acute toxicity log Kow cutoff: 5.0  
 Green algal EC50 toxicity log Kow cutoff: 6.4  
 Chronic toxicity log Kow cutoff: 8.0  
 MW cutoff: 1000



SMILES : OCCOCCOC(=O)C1(C)C2CC=C3C=C(C(C)C)CCC3C2(C)CC1  
 CHEM :  
 MOL FOR : C24 H38 O4  
 MOL WT : 390.57

----- EPI SUMMARY (v3.10) -----

Physical Property Inputs:

Water Solubility (mg/L):	-----	Log Kow (oct-water):	6.03
Vapor Pressure (mm Hg):	-----	Boiling Pt (deg C):	-----
Henry LC (atm-m3/mole):	-----	Melting Pt (deg C):	25.00

Log Kow (KOWWIN v1.66 estimate) = 5.50

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.40):

Boiling Pt (deg C): 452.20  
 Melting Pt (deg C): 181.06  
 VP(mm Hg,25 deg C): 5.23E-009

Water Solubility estimate (WSKOW v1.40): 0.4938 mg/L

Henrys Law Constant (atm-m3/mole) [HENRYWIN v3.10]:

Bond Method: 1.63E-009 Group Method: Incomplete  
 Henrys LC [VP/WSol estimate using EPI values]: 5.443E-009 atm-m3/mole

Biodegradation Estimates (BIOWIN v4.00):

Linear Model: 0.1793 Non-Linear Model: 0.0145  
 Ultimate Model: 2.2033 (months) Primary Model: 3.3260 (days-weeks)  
 Linear MITI: 0.4960 Non-Linear MITI: 0.1551

Atmospheric Oxidation (25 deg C) [AopWin v1.90]:

OH Half-Life = 0.036 Days (12-hr day; 1.5E6 OH/cm3)  
 Ozone Half-Life = 0.001 Days (at 7E11 mol/cm3)

Soil Adsorption (PCKOCWIN v1.66): Koc = 4132 Log Koc = 3.616

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:

Kb Half-Life at pH 7: 8.810 years

BCF estimate (BCFWIN v2.14): Log BCF = 3.943 (BCF = 8772)

Volatilization from Water: (Henry LC = 1.63e-009 atm-m3/mole)

Half-Lives: Model River = 7.099e+005 hr, Model Lake = 7.744e+006 hr

Removal In Wastewater Treatment (percents):

TOTAL: 92.28, Biodeg: 0.77, Sludge: 91.51, Air: 0.00

Level III Fugacity Model (conc %, half-life hr):

Air(0.00062%,0.0267), Water(5.11%,1.44e+003), Soil(33.6%,1.44e+003), Sediment(61.3%,5.76e+003)  
 Persistence Time: 2.06e+003 hr

-----  
 CHEMICAL: Unknown 09:59:55 12/06/:4  
 MOL WT : 390.57  
 MOL FOR: C24H38O4  
 SMILES : OCCOCCOC(=O)C1(C)C2CC=C3C=C(C(C)C)CCC3C2(C)CCC1  
 ISOC-ID: -AA-AA-----A--A-A-AV-V-V-V-A-A-A-AAA-A--A-AAA-  
 FRAG-ID: 1 2 33 3  
 H-COUNT: 122 22 3 1 21 1 1 3 3 221 3 222  
 -----

Class	Type	Contribution Description	Comment	Value
FRAGMENT	# 1	Alcohol or Hydroxy	MEASURED	-1.640
FRAGMENT	# 2	Ether	MEASURED	-1.820
FRAGMENT	# 3	Ester	MEASURED	-1.490
ISOLATING	CARBON	23 Aliphatic isolating carbon(s)		4.485
EXFRAGMENT	BRANCH	4 chain and 4 cluster branch(es)	(COMBINED)	-1.040
EXFRAGMENT	BRANCH	1 Non-halogen, polar group branch(es)	(Group)	-0.220
EXFRAGMENT	HYDROG	37 Hydrogen(s) on isolating carbons		8.399
EXFRAGMENT	BONDS	8 chain and 16 alicyclic (net)	(COMBINED)	-2.400
PROXIMITY	Y-CC-Y	1 pairs over bond 3- 2 (AvWt=-.260)		0.900
PROXIMITY	Y-CC-Y	1 pairs over bond 6- 5 (AvWt=-.260)		0.861
RESULT	v3.3	All fragments measured	ESTIMATE	6.034