

Test Material: Telone

MRID: 44536501
Title: Method Validation Report for GRM 94.18 - Determination of Residues of *cis*- and *trans*-3-Chloroallyl Alcohol in Soil by Capillary Gas Chromatography with Mass Selective Detection

MRID: 44536502
Title: Independent Laboratory Validation of Method GRM 94.18 - Determination of Residues of *cis*- and *trans*-3-Chloroallyl Alcohol in Soil by Capillary Gas Chromatography with Mass Selective Detection

EPA PC Code: 029001

OCSPP Guideline: 850.6100

For CDM Smith

Primary Reviewer: Lynne Binari

Signature:



Date: 6/15/15

Secondary Reviewer: Lisa Muto

Signature:



Date: 6/15/15

QC/QA Manager: Joan Gaidos

Signature:



Date: 6/15/15

Analytical method for telone transformation products cis- and trans-3-chloroallyl alcohol in soil

Reports: ECM: EPA MRID No.: 44536501. Duebelbeis, D.O., and A.D. Thomas. 1997. Method Validation Report for GRM 94.18 - Determination of Residues of *cis*- and *trans*-3-Chloroallyl Alcohol in Soil by Capillary Gas Chromatography with Mass Selective Detection. Report prepared, sponsored, and submitted by Global Environmental Chemistry Laboratory - Indianapolis Lab, DowElanco, Indianapolis, Indiana; 44 pages. DowElanco Study ID: RES94140. Final report issued December 12, 1997.
ILV: EPA MRID No. 44536502. Duebelbeis, D.O., K. Hostetler, and B.J. Markley. 1996. Independent Laboratory Validation of Method GRM 94.18 - Determination of Residues of *cis*- and *trans*-3-Chloroallyl Alcohol in Soil by Capillary Gas Chromatography with Mass Selective Detection. Report prepared by Global Environmental Chemistry Laboratory - Indianapolis Lab, DowElanco, Indianapolis, Indiana, and Wildlife International Ltd., Easton, Maryland, sponsored and submitted by Global Environmental Chemistry Laboratory - Indianapolis Lab, DowElanco, Indianapolis, Indiana; 34 pages. Wildlife International Project No.: 379C-117. DowElanco Project No. and Study ID: RES95082. Final report issued August 2, 1996.

Document No.: MRIDs 44536501 & 44536502

Guideline: 850.6100

Statements: ECM: The study was conducted in compliance with USEPA Good Laboratory Practice (GLP) standards, with minor exceptions (p. 3 of MRID 44536501). Signed and dated Data Confidentiality, GLP, and Quality Assurance statements were provided (pp. 2-4). The certification of the authenticity of the study report is included in the Quality Assurance Statement (p. 4).
ILV: The study was conducted in compliance with USEPA GLP standards (p. 3 of MRID 44536502). Signed and dated Data Confidentiality, GLP, and Quality Assurance statements were provided (pp. 2-4). The certification of the authenticity of the study report is included in the Quality Assurance Statement (p. 4).

Classification: This analytical method is classified as unacceptable. The ILV was not conducted independently of the ECM originating laboratory. Though the ILV was conducted at a different laboratory, the ECM and ILV are conducted by the same study director. The experimental design of the ILV was inadequate to produce a successful validation of the ECM, with insufficient performance data at the LOQ (n = 2) and no performance data at 10x LOQ. For both the ECM and ILV, soil matrices were not characterized. The registrant failed to verify that the independent laboratory performed the ILV with a soil of the most difficult analytical sample condition to analyze to demonstrate how well the method performs. The ILV did not verify the LODs for the analytes. For the ILV, sample recoveries were corrected for residues detected in the matrix control samples. For the ECM, performance data at 10x LOQ were not reported.

PC Code: 029001

Reviewer:

Andrew Shelby, Physical Scientist

Signature: **Date:** May 10, 2016

For both MRIDs, page citations in this review refer to the uppermost set of page numbers located in the top right corner of each page of the MRID.

Executive Summary

DowElanco Analytical Method GRM 94.18 is designed for the quantitative determination of telone transformation products cis- and trans-3-chloroallyl alcohol (CAAL, derivatized to the respective 3-chloroallyl isobutyl carbonate) in soil using GC/MS. The method is quantitative for the analytes at the stated LOQ of 0.42 ng/g ($\mu\text{g}/\text{kg}$). The LOQ is less than the lowest toxicological level of concern in soil (Earthworm 14-day $\text{LC}_{50} = 55.6\text{mg}/\text{kg}$ for 1,3-D from PPDB). No major modifications were made by the independent laboratory. The independent laboratory failed to validate the method for analysis of cis- and trans-3-CAAL in soil (uncharacterized) because insufficient performance data were reported at the LOQ ($n = 2$) and no performance data were reported at 10x LOQ. The ILV did not verify the LODs for the analytes. The ECM validation did not provide performance data at 10x LOQ. For both the ECM and ILV, soil matrices were not characterized. The registrant failed to verify that the independent laboratory performed the ILV with a soil of the most difficult analytical sample condition to analyze to demonstrate how well the method performs. The ILV was not conducted independently of the ECM originating laboratory.

Table 1. Analytical Method Summary

Analyte(s) by Pesticide	MRID		EPA Review	Matrix	Method Date (dd/mm/yyyy)	Registrant	Analysis	Limit of Quantitation (LOQ)
	Environmental Chemistry Method	Independent Laboratory Validation						
cis-3-CAAL ¹	44536501	44536502		Soil ²	15/03/1995 ³	DowElanco	GC/MS	0.42 ng/g ($\mu\text{g}/\text{kg}$)
trans-3-CAAL								

1 CAAL = chloroallyl alcohol; transformation product of telone.

2 Uncharacterized in the ECM validation and ILV. Soil for ECM validation obtained near Immokalee, Florida (p. 8 of MRID 44536501). Source location for soil used in ILV was not reported.

3 Appendix A, p. 15 of MRID 44536501.

I. Principle of the Method

Soil (10.0 g) was fortified with cis- and trans-3-chloroallyl alcohol (CAAL) in acetone for procedural recoveries (p. 9; Appendix A, pp. 19-20, 22 of MRID 44536501). Uncharacterized soil from a site near Immokalee, Florida, was used for the validation (p. 8). Soil samples (10.0 g) are extracted twice with 15.0 mL of 0.01N hydrochloric acid by shaking (reciprocating shaker, *ca.* 180 excursion/minute) for ≥ 30 minutes for each extraction (Appendix A, p. 22). Soil and extract are separated by centrifugation (2,500 rpm, 10 minutes), with the extracts decanted and combined. The combined extract is applied to an ion-exchange (quaternary amine) solid phase extraction (SPE) column equipped with a pre-filter (glass fiber Acrodisc) and pre-conditioned with methanol and deionized water (Appendix A, pp. 17-18, 22-23). The sample is pulled through the column by vacuum (*ca.* 2 mL/minute), with eluate collection. The extract sample flask is rinsed twice with deionized water (3 mL x 2), with rinsates applied to the SPE column and all collected eluates combined. The sample is partitioned with 15 mL of methyl-t-butyl ether (MTBE), 15 g of sodium chloride, and 10 μL of 1-propanol by shaking (as described above) for 15 minutes (1-propanol is critical to reduce evaporative losses of CAAL; Appendix A, pp. 18, 23). Phases are separated by centrifugation (1,000 rpm, 3 minutes). The organic (MTBE) phase is applied, through anhydrous

magnesium sulfate (*ca.* 2 g), to a silica gel SPE column preconditioned with MTBE. The sample is pulled through the column by vacuum (*ca.* 2 mL/minute), with eluate collection. The remaining aqueous phase is again partitioned with 15 mL of MTBE by shaking for 5 minutes and the resulting organic phase applied to the silica gel SPE column, with all eluates combined. The sample is combined with hexane (*ca.* 3 mL) and anhydrous sodium sulfate (*ca.* 0.1 g), then taken to near dryness using a flask equipped with a Micro Snyder distilling column on a hot plate (Appendix A, pp. 18, 24). Residues are reconstituted with hexane (*ca.* 1 mL) and concentrated to *ca.* 0.5 mL under a gentle nitrogen stream (N-Evap, ambient temperature). Residues are reconstituted to 1.0 mL with hexane, amended with anhydrous sodium sulfate (*ca.* 0.1 g), then derivatized to the respective cis- and trans-3-chloroallyl isobutyl carbonates (CAIBC) with isobutyl chloroformate (25 μ L) in the presence of pyridine (25 μ L) at 70°C for 15 minutes (Appendix A, pp. 15, 24). Upon cooling, samples are treated with 1.0 mL of 0.1N hydrochloric acid, vortexed (5 seconds), centrifuged (2,500 rpm, 5 minutes), and the upper hexane layer taken for GC/MS analysis.

Samples are analyzed using an Hewlett-Packard 5971A Mass Selective Detector (MSD) equipped with an Hewlett-Packard 5890 (II) GC system (Appendix A, p. 21 of MRID 44536501). The following GC conditions were used: J&W Scientific fused silica capillary, Durabond-17 (DB-17) liquid phase column (0.18 mm x 20 m, 0.3 μ m film thickness, injector temperature 230°C), temperature program [65°C (hold for 1 min.), 5°C/min. to 150°C (0 min. hold), 20°C/min. to 260°C (0 min. hold)]. Injection volume was 2 μ L. The following MSD conditions were used: electron impact ionization and selected ion monitoring (SIM). Analytes were identified using two ions; one for quantitation (Q) and one for confirmation (C). Ions monitored were m/z 136 (Q) and m/z 75 (C) for both cis- and trans-3-CAIBC. Identification is considered positive when the confirmation ion ratio [(peak area at m/z 136)/(peak area at m/z 75)] of the sample is \pm 20% of the average confirmation ion ratio found for the calibration standards (Appendix A, p. 25). Retention times for cis- and trans-3-CAAL (as CAIBC) were 13.41-13.42 and 13.27 minutes, respectively (Appendix A, Figure 5, p. 39; Figures 7-8, pp. 41-42; Figure 10, p. 44).

ILV: Sources of the test compounds and soil matrix used for the ILV were not reported (p. 9; Appendix A, p. 31 of MRID 44536502). The soil matrix was not characterized. The independent laboratory performed the extraction method as written, with one equipment substitution (Multivap Analytical evaporator for the N-Evap; pp. 10-12). Retention times for cis- and trans-3-CAAL (as CAIBC) were 13.95-13.96 and 13.76-13.80 minutes, respectively (Figures 3-8, pp. 22-27).

LOQ and LOD: In the ECM and ILV, the LOQ for both cis- and trans-3-CAAL was 0.42 ng/g (μ g/kg; Appendix A, p. 15 of MRID 44536501; p. 9 of MRID 44536502). In the ECM, the LODs for cis- and trans-3-CAAL were calculated as 0.13 ng/g and 0.11 ng/g, respectively (p. 11; Appendix A, pp. 28-29; Tables III-IV, pp. 33-34 of MRID 44536501). In the ILV, the LODs were not specified.

II. Recovery Findings

ECM (MRID 44536501): Mean recoveries and relative standard deviations (RSDs) were within guidelines (mean 70-120%; RSD \leq 20%) for analysis of cis- and trans-3-CAAL in a Florida soil (uncharacterized) at a fortification level of 0.42 ng/g ($\mu\text{g}/\text{kg}$, LOQ, n = 9; Appendix A, Tables I-II, pp. 31-32 and DER Attachment 2). At fortification levels of 2.5x (1.039-1.043 ng/g), 5x (2.078-2.086 ng/g), 25x (10.39-10.43 ng/g), 50x (20.78-20.86 ng/g), 250x (103.9-104.3 ng/g), 1,250x (519.5-521.5 ng/g), and 5,000x (2,078-2,086 ng/g) LOQ, only two recoveries were reported for each fortification level; therefore, meaningful statistics (mean, standard deviation, RSD) for the recovery results per analyte/fortification level/soil matrix could not be generated. At the fortification levels of 2.5x to 5,000x LOQ, individual recovery results were within 70-120%. Performance data at 10x LOQ were not reported. Confirmation ion ratio results were only provided for one LOQ (0.42 ng/g) fortified sample for both cis- and trans-3-CAAL and were \pm 5% of the average standard confirmation ratio (Appendix A, Figure 7, p. 41; Figure 10, p. 44).

ILV (MRID 44536502): Only two recoveries were reported for each fortification level; therefore, meaningful statistics (mean, standard deviation, RSD) for the recovery results per analyte/fortification level/soil matrix could not be generated. Individual recovery results were within 70-120% for both cis- and trans-3-CAAL in soil (uncharacterized) at fortification levels of 0.42 ng/g (LOQ) and 2.1 ng/g (5x LOQ; Tables I-II, pp. 17-18). Performance data at 10x LOQ were not reported. Confirmation ion ratio results were only provided for one LOQ (0.42 ng/g) fortified sample for both cis- and trans-3-CAAL and were \pm 5% of the average standard confirmation ratio (Figure 5, p. 24; Figure 8, p. 27). One validation run was conducted and considered successful (p. 16).

Table 2. Initial Validation Method Recoveries for Telone Transformation Products cis- and trans-3-Chloroallyl Alcohol (CAAL) in Soil¹

Analyte	Fortification Level (ng/g)	Number of Tests	Recovery Range (%)	Mean Recovery (%)	Standard Deviation (%)	Relative Standard Deviation (%)
cis-3-CAAL	0.42 (LOQ) ²	9	71-106	88	10	12
	1.043	2	98, 91	-- ³	--	--
	2.086	2	83, 75	--	--	--
	10.43	2	77, 87	--	--	--
	20.86	2	90, 94	--	--	--
	104.3	2	77, 78	--	--	--
	521.5	2	78, 84	--	--	--
	2086	2	83, 92	--	--	--
trans-3-CAAL	0.42 (LOQ) ⁴	9	76-105	90	9	10
	1.039	2	95, 93	--	--	--
	2.078	2	86, 77	--	--	--
	10.39	2	79, 89	--	--	--
	20.78	2	92, 98	--	--	--
	103.9	2	82, 84	--	--	--
	519.5	2	81, 88	--	--	--
	2078	2	86, 95	--	--	--

Data (uncorrected recovery results) were obtained from Appendix A, Tables I-II, pp. 31-32 of MRID 44536501 and DER Attachment 2 (mean, SD, RSD).

1 Uncharacterized soil collected from a site near Immokalee, Florida (p. 8).

2 Fortification level was 0.4172 ng/g (Appendix A, Table I, p. 31). Two fortifications made at 0.0834 ng/g (20% of LOQ) had recoveries of 108% (0.090 ng/g) and 54% (0.045 ng/g).

3 Not applicable; meaningful statistics could not be generated because n = 2.

4 Fortification level was 0.4156 ng/g (Appendix A, Table II, p. 32). Two fortifications made at 0.0831 ng/g (20% of LOQ) had recoveries of 112% (0.093 ng/g) and 61% (0.051 ng/g).

Table 3. Independent Validation Method Recoveries for Telone Transformation Products cis- and trans-3-Chloroallyl Alcohol (CAAL) in Soil¹

Analyte	Fortification Level (ng/g)	Number of Tests	Recovery Range (%)	Mean Recovery (%)	Standard Deviation (%)	Relative Standard Deviation (%)
cis-3-CAAL	0.42 (LOQ)	2	90, 83	-- ²	--	--
	2.1	2	90, 86	--	--	--
trans-3-CAAL	0.42 (LOQ)	2	83, 71	--	--	--
	2.1	2	90, 86	--	--	--

Data (recovery results, corrected for any residues detected in matrix control samples) were obtained from Tables I-II, pp. 17-18; Figure 5, p. 24; Figure 8, p. 27 of MRID 44536502.

1 Uncharacterized; source location was not reported.

2 Not applicable; meaningful statistics could not be generated because n = 2.

III. Method Characteristics

In the ECM and ILV, the LOQ for both cis- and trans-3-CAAL was 0.42 ng/g ($\mu\text{g}/\text{kg}$; Appendix A, p. 15 of MRID 44536501; p. 9 of MRID 44536502). In the ECM, the LODs for cis- and trans-3-CAAL were calculated as 0.13 ng/g and 0.11 ng/g, respectively (p. 11; Appendix A, pp. 28-29; Tables III-IV, pp. 33-34 of MRID 44536501). In the ILV, the LODs were not specified. Following the method of Keith, L.H., *et al.* (see section V. **References** below), the LOD and LOQ for determination of telone transformation products cis- and trans-3-chloroallyl alcohol in soil were calculated using the standard deviation from the 0.42 ng/g (LOQ) recovery results (Appendix A, pp. 28-29; Tables III-IV, pp. 33-34 of MRID 44536501). The LOD was calculated as three times the standard deviation ($3s$), and the LOQ was calculated as ten times the standard deviation ($10s$) of the recovery results. Matrix blank values ($n = 6$) were 0.0000 ng/g (Appendix A, Tables I-II, pp. 31-32). Calculated LOQ values were 0.42 ng/g and 0.36 ng/g for cis- and trans-CAAL, respectively.

Table 4. Method Characteristics for Telone Transformation Products cis- and trans-3-Chloroallyl Alcohol (CAAL)¹ in Soil

		cis-3-CAAL	trans-3-CAAL
Limit of Quantitation (LOQ)		0.42 ng/g ($\mu\text{g}/\text{kg}$)	
Limit of Detection (LOD)		0.13 ng/g	0.11 ng/g
Linearity (calibration curve r^2 and concentration range) ²	ECM:	Q ion: $r^2 = 0.9994$ (0.2086-41.72 ng/g in soil)	Q ion: $r^2 = 0.9996$ (0.2078-41.56 ng/g in soil)
	ILV:	Q ion: $r^2 = 0.997$ (0.20-10.0 ng/g in soil)	Q ion: $r^2 = 0.997$ (0.20-10.0 ng/g in soil)
Repeatable	ECM:	Yes at LOQ ($n = 9$). No performance data at 10x LOQ. All other fortification levels, 2.5x to 5,000x LOQ, performed at $n = 2$.	
	ILV:	Undetermined. Fortifications at LOQ and 5x LOQ performed at $n = 2$. No performance data at 10x LOQ.	
Reproducible		Undetermined. ILV performed at $n = 2$ at LOQ and 5x LOQ.	
Specific ³	ECM:	Yes, no interferences were detected at analyte retention times (Appendix A, Figure 6, p. 40; Figure 9, p. 43). Matrix was uncharacterized Florida soil.	
	ILV:	No interferences detected at analyte retention times for Q ion (m/z 136), but interferences of 25-28% of the LOQ were detected with the C ion (m/z 75; Figures 4-5, pp. 23-24; Figures 7-8, pp. 26-27). Matrix was uncharacterized soil; source location was not reported.	

Data were obtained from pp. 8, 11; Appendix A, p. 15; Tables I-IV, pp. 31-34; Figures 3-4, pp. 37-38; Figure 6, p. 40; Figure 9, p. 43 of MRID 44536501; p. 9; Tables I-II, pp. 17-18; Figures 1-2, pp. 20-21; Figures 4-5, pp. 23-24; Figures 7-8, pp. 26-27 of MRID 44536502.

Linearity is satisfactory when $r^2 \geq 0.995$.

¹ Derivatized as cis- and trans-3-chloroallyl isobutyl carbonate (CAIBC; Appendix A, p. 15 of MRID 44536501).

² Calibration curve r^2 values determined using power regression equation (Appendix A, Figures 3-4, pp. 37-38 of MRID 44536501; Figures 1-2, pp. 20-21 of MRID 44536502).

³ For both the ECM validation and ILV, confirmation ion ratio results were only provided for one LOQ (0.42 ng/g) fortified sample for both cis- and trans-3-CAAL and were $\pm 5\%$ of the average standard confirmation ratio (Appendix A, Figure 7, p. 41; Figure 10, p. 44 of MRID 44536501; Figure 5, p. 24; Figure 8, p. 27 of MRID 44536502). A confirmatory method is typically not required where GC/MS and LC/MS methods are used as the primary method.

IV. Method Deficiencies and Reviewer's Comments

1. The ILV was not conducted independently of the ECM originating laboratory. The study director of the ECM validation, and author of the method and ECM validation study report, D.O. Duebelbeis, was also the study director of the ILV and co-author of the ILV study report (pp. 1, 3, 5; Appendix A, p. 15 of MRID 44536501; pp. 1, 3, 5 of MRID 44536502).
2. The experimental design of the ILV was inadequate to produce a successful validation of the ECM. For the ILV, only two recoveries were reported for both the LOQ and 5x LOQ fortification levels, with no performance data at 10x LOQ (Tables I-II, pp. 17-18 of MRID 44536502). A validation sample set should consist of, at a minimum, a reagent blank, two unspiked matrix control samples, five matrix control samples spike at the LOQ, and five matrix control samples spiked at 10x LOQ for each analyte and matrix.
3. For both the ECM validation and ILV, the soil matrices were not characterized. In the ECM, the soil sample numbers were M465A, M465B and M465E (Tables I-IV, pp. 31-34 of MRID 44536501); in the ILV, the soil identification number was M465B (Appendix A, p. 31 of MRID 44536502). These soil matrices were characterized as sand soils by A & L Great Lakes Laboratories, Inc., Fort Wayne, Indiana in concurrent MRIDs (Appendix C, pp. 83, 85 of MRID 44536504; Appendix C, pp. 117-118 of MRID 44536511). The registrant failed to verify that the independent laboratory performed the ILV with a soil of the most difficult analytical sample condition to analyze to demonstrate how well the method performs.
4. The ILV did not verify the LODs for the analytes as determined by the ECM validation.
5. For the ILV, sample recoveries were corrected when residues were found in the matrix control samples (pp. 13-14; Figure 5, p. 4; Figure 8, p. 27 of MRID 44536502).
6. For the ECM validation, performance data at 10x LOQ were not reported. At fortification levels >LOQ (2.5x to 5,000x LOQ), only two recoveries were reported at each fortification level (Appendix A, Tables I-II, pp. 31-32 of MRID 44536501).
7. For the ILV, chromatograms for reagent blank and 2.1 ng/g (5x LOQ) spiked samples were not provided (Figures 4-5, pp. 23-24; Figures 7-8, pp. 26-27 of MRID 44536502). For the calibration standards, only chromatograms of 0.20 ng/g (in soil, 2.0 ng/mL standard) cis- and trans-3-CAAL standards were provided (calibration standard range 0.20-10.0 ng/g in soil; Figures 1-3, pp. 20-22; Figure 6, p. 25).

For both cis- and trans-3-CAAL, interferences of 25-28% of the LOQ were observed with the confirmatory ion (m/z 75; Figures 4-5, pp. 23-24; Figures 7-8, pp. 26-27).

8. For the ECM validation, chromatograms for reagent blank and spiked samples, other than LOQ, were not provided (Appendix A, Figures 6-7, pp. 40-41; Figures 9-10, pp. 43-44 of MRID 44536501). For the calibration standards, only chromatograms of 0.42 ng/g (in soil, 4.2 ng/mL standard) cis- and trans-3-CAAL standards were provided (calibration standard range 0.21-42 ng/g in soil; Appendix A, Figures 3-5, pp. 37-39; Figure 8, p. 42).

In the ECM study report, the study authors described r^2 as both correlation coefficient and coefficient of determination (p. 10; Appendix A, p. 28; Figures 3-4, pp. 37-38). The reviewer verified that the r^2 values reported in the ECM and ILV study reports are coefficients of determination (r^2 ; DER Attachment 2).

9. It was reported for the ILV that a set of seven samples (one reagent blank, two matrix controls, and four fortified samples) required *ca.* 12 person hours (1.5 calendar days) to complete (p. 16; Appendix A, p. 33 of MRID 44536502).

V. References

Keith, L.H.; Crummett, W.B.; Deegan, J.; Libby, R.A.; Taylor, J.T.; Wentler, G., "Principles of Environmental Analysis", *Anal. Chem.*, 1983, **55**, pp. 2210-2218 (Appendix A, p. 30 of MRID 44536501).

U.S. Environmental Protection Agency. 2012. Ecological Effects Test Guidelines, OCSPP 850.6100, Environmental Chemistry Methods and Associated Independent Laboratory Validation. Office of Chemical Safety and Pollution Prevention, Washington, DC. EPA 712-C-001.

40 CFR Part 136. Appendix B. Definition and Procedure for the Determination of the Method Detection Limit-Revision 1.11, pp. 317-319.

Attachment 1: Chemical Names and Structures**cis- and trans-3-Chloroallyl alcohol (CAAL)**

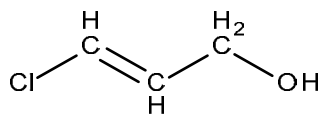
IUPAC Name: (E_Z)-3-chloroprop-2-en-1-ol
cis-: (Z)-3-chloroprop-2-en-1-ol
trans-: (E)-3-chloroprop-2-en-1-ol

CAS Name: 3-Chloro-2-propen-1-ol

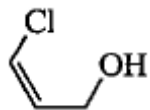
CAS Number: 29560-84-7
cis- : 4643-05-4
trans- : 4643-06-5

SMILES String: C(/C=C/Cl)O

3-CAAL



cis-3-CAAL



trans-3-CAAL

