

Test Material: Methiocarb

MRID: 49502503

Title: Development and Validation of a Method for the Determination of Methiocarb, Methiocarb Sulfoxide and Methiocarb Sulfone in Water

MRID: 49519606

Title: INDEPENDENT LABORATORY VALIDATION OF METHODS FOR THE DETERMINATION OF METHIOCARB AND ITS METABOLITES METHIOCARB SULFOXIDE AND METHIOCARB SULFONE IN SURFACE WATER BY LC/MS/MS

EPA PC Code: 100501

OCSPP Guideline: 850.6100

For CDM Smith

Primary Reviewer: Lisa Muto

Signature:



Date: 7/14/15

Secondary Reviewer: Lynne Binari

Signature:



Date: 7/14/15

QC/QA Manager: Joan Gaidos

Signature:



Date: 7/14/15

Analytical method for methiocarb sulfoxide and its transformation products methiocarb sulfoxide and methiocarb sulfone in water

Reports: ECM: EPA MRID No.: 49502503. Shen, H. 2014. Development and Validation of a Method for the Determination of Methiocarb, Methiocarb Sulfoxide and Methiocarb Sulfone in Water. PTRL Study No.: 2465W. Report prepared by PTRL West (a division of EAG, Inc.), Hercules, California; sponsored and submitted by Gowan Company, Yuma, Arizona; 76 pages. Final report issued August 19, 2014.
ILV: EPA MRID No. 49519606. MacGregor, J.A, and E.S. Bodle. 2014. INDEPENDENT LABORATORY VALIDATION OF METHODS FOR THE DETERMINATION OF METHIOCARB AND ITS METABOLITES METHIOCARB SULFOXIDE AND METHIOCARB SULFONE IN SURFACE WATER BY LC/MS/MS. Wildlife International Project No.: 334C-121. Report prepared by Wildlife International, Evans Analytical Group, Easton, Maryland, sponsored and submitted by Gowan Company, Yuma, Arizona; 163 pages. Final report issued November 25, 2014.

Document No.: MRIDs 49502503 & 49519606


Guideline: 850.6100

Statements: ECM: EPA MRID No.: 49502503. The study was conducted in accordance with USEPA GLP standards (40 CFR 160), with the exception that the certificates of analysis of the methiocarb sulfoxide and methiocarb sulfone reference substances may or may not have been GLP certified (p. 3). Signed and dated No Data Confidentiality, GLP, and Quality Assurance statements were provided (pp. 2-4). A statement of the authenticity of the study report was included with the QA statement.
ILV: EPA MRID No. 49519606. The study was conducted in accordance with USEPA FIFRA, OECD and Japanese GLP standards, with the exception of the storage stability characterization and testing (p. 3). Signed and dated No Data Confidentiality, GLP, and Quality Assurance statements were provided (pp. 2-4). A statement of the authenticity of the study report was not included.

Classification: This analytical method is classified as Unacceptable/Upgradable. The determinations of the LOQ and LOD were not based on scientifically acceptable procedures. The LOD was not reported in the ILV. In the ECM, method recoveries of methiocarb sulfoxide and methiocarb sulfone at the LOQ did not meet OCSPP Guideline 850.6100 criteria for precision and accuracy. A reagent blank was not included in the ILV.

PC Code: 100501

EPA Primary Reviewer: James C. Hook III
Ecologist

Signature: 
Date: March 7, 2016

EPA Secondary Reviewer: William P. Eckel, Ph.D
Senior Science Advisor

Signature: 
Date: March 7, 2016

Executive Summary

This analytical method, PTRL Study No. 2465W, is designed for the quantitative determination of methiocarb and its transformation products methiocarb sulfoxide and methiocarb sulfone in water at 0.1 ppb using LC/MS/MS. The ILV found the method quantitative for the analytes at the stated LOQ of 0.1 ppb; however, ECM validation method recoveries of methiocarb sulfoxide (RSDs of 25% for quantitation and confirmation ions) and methiocarb sulfone (RSDs of 42% and 38% for quantitation and confirmation ions, respectively) at the LOQ did not meet OCSPP Guideline 850.6100 criteria for precision and accuracy (mean 70-120%, RSD \leq 20%). The LOQ is equal to the lowest toxicological level of concern in water. Although the number of trials was not reported, the reviewer assumed that the ILV validated the method in the first trial. Both the ECM and ILV validated the method using surface water.

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						
Methiocarb	49502503	49519606		Water	19/08/2014	Gowan Company	LC/MS/MS	0.1 ppb (0.100 μ g/L)
Methiocarb sulfoxide								
Methiocarb sulfone								

I. Principle of the Method

Samples (100 mL) of water were fortified (0.100 mL of 100 ng/mL or 1 μ g/mL mixed fortification solution), as necessary, then extracted with 50 mL of methylene chloride and 1 g of sodium chloride by shaking vigorously in a separatory funnel for 2 minutes (pp. 20-22; Figure 1, p. 35 of MRID 49502503). The organic layer was transferred to a concentration flask. The aqueous layer was extracted with 50 mL of ethyl acetate by shaking vigorously for 2 minutes. The upper organic layer was combined with that of the previous extraction. The aqueous layer was returned to the separatory funnel. The container for the aqueous layer was rinsed with 50 mL of ethyl acetate, which was then added to the separatory funnel. The aqueous layer was extracted again with shaking vigorously for 2 minutes. The organic layer was combined with the previous extracts. The separatory funnel was rinsed with 5 mL of methylene chloride. The combined extracts and rinses were concentrated to *ca.* 5 mL using a rotary evaporator at 30°C. The residue was transferred to a 15-mL disposable glass tube using 5 mL of ethyl acetate. The residue was concentrated to *ca.* 0.2 mL via turbo evaporator under nitrogen at 30°C then further evaporated to dryness manually under nitrogen. The final residue was reconstituted with 1.0 mL methanol via sonication prior to LC/MS/MS analysis.

Samples were analyzed for methiocarb, methiocarb sulfoxide and methiocarb sulfone using a Thermo Scientific Dionex Ultimate 3000 Liquid Chromatograph coupled to an AB Sciex API 4000 Triple Quad Mass Spectrometer (MRM; pp. 18, 23-24 of MRID 49502503). The instrumental conditions consisted of an Agilent Zorbax® SB-CN column (4.6 x 75 mm, 3.5- μ m; column temperature unreported), a mobile phase gradient of (A) water containing 0.05% formic acid and (B) methanol containing 0.05% formic acid [percent A:B (v:v) at 0.0-0.5 min. 80:20, 4.0-6.5 min. 10:90, 7.0-12.5 min. 80:20] and MS/MS detection in APCI positive mode (temperature, 300°C). Two parent-daughter ion transitions (quantitative = Q, confirmatory = C) were monitored: m/z 226 \rightarrow 169 (Q) and m/z 226 \rightarrow 121 (C) for methiocarb; m/z 242 \rightarrow 185 (Q) and m/z 242 \rightarrow 170 (C) for methiocarb sulfoxide; and m/z 258 \rightarrow 107 (Q) and m/z 258 \rightarrow 202 (C) for methiocarb sulfone (p. 24; Appendix D, pp. 74-76). Approximate retention times were *ca.* 6.20-6.22 min., *ca.* 5.07-5.09 min. and *ca.* 5.38-5.41 min. for methiocarb, methiocarb sulfoxide and methiocarb sulfone, respectively (Figures 13-14, pp. 54-59). Injection volume was 10 μ L (p. 23)

ILV

In the ILV, the ECM extraction method was performed exactly as written (pp. 15-16; Appendix II, pp. 75-151 of MRID 49519606). The analytical method was performed as described in the ECM method using an Agilent Technologies 1260 HPLC coupled to an AB Sciex Triple QUAD 5500 Mass Spectrometer (Turbo-V Ion Spray Source; p. 16; Table 1, p. 21). Approximate retention times for the analytes were *ca.* 6.9 min., *ca.* 5.8 min. and *ca.* 6.1 min. for methiocarb, methiocarb sulfoxide and methiocarb sulfone, respectively. For methiocarb sulfone, the monitored confirmation ion transitions differed slightly from that reported in the ECM: m/z 258 \rightarrow 201 (C).

LOQ/LOD

The Limit of Quantification (LOQ) and Limit of Detection (LOD) for all analytes were reported as 0.1 ppb and 0.02 ppb (20% of the LOQ), respectively, in the ECM (p. 25 of MRID 49502503). The LOQ and LOD represented 10 ng/mL and 2 ng/mL in solution, respectively. In the ILV, only the LOQ (0.100 μ g/L) was reported (p. 13 of MRID 49519606).

II. Recovery Findings

ECM (MRID 49502503): Mean recoveries and relative standard deviations (RSDs) met requirements (mean 70-120%; RSD \leq 20%) for analysis of methiocarb in surface water at the LOQ (0.1 ppb) and 10 \times LOQ (1 ppb) and for methiocarb sulfoxide and methiocarb sulfone in surface water at 10 \times LOQ (1 ppb; Table I, pp. 32-33). Including all replicate data, recoveries of methiocarb sulfoxide and methiocarb sulfone at the LOQ (0.1 ppb) did not meet requirements with RSDs of 25% for both the quantitation and confirmation ions for methiocarb sulfoxide and 42% and 38% for the quantitation and confirmation ions, respectively, for methiocarb sulfone (Appendix D, pp. 75-76; DER Attachment 2). For both methiocarb sulfoxide and methiocarb sulfone at the LOQ, the study author excluded the recovery data of one replicate from the statistics as it was determined to be an outlier based on Dixon's Q test at the 99% confidence level: 58% and 56% for methiocarb sulfoxide and 23% and 29% for methiocarb sulfone (quantitative and confirmation ion, respectively Appendix D, pp. 75-76). Analytes were identified and quantified using two ion transitions; quantification and confirmation ion results were comparable. The surface water was collected from Richmond, California (Inventory No. 2465W-004; source not further specified; p. 18). The water matrix was characterized by Agvise Laboratories, Northwood, North Dakota (p. 19; Appendix C, p. 73).

ILV (MRID 49519606): Mean recoveries and relative standard deviations (RSDs) met requirements (mean 70-120%; RSD \leq 20%) for analysis of methiocarb, methiocarb sulfoxide and methiocarb sulfone in surface (lake) water at the LOQ (0.1 ppb) and 10 \times LOQ (1 ppb; Tables 2-7, pp. 22-27). Analytes were identified and quantified using two ion transitions; quantification and confirmation ion results were comparable. The surface water was collected from Tuckahoe Lake in Tuckahoe State Park, Ridgely, Maryland (Inventory No. 2465W-004; p. 13). The water matrix was characterized by Agvise Laboratories, Northwood, North Dakota (Appendix III, p. 152). The number of trials was not specified, but the reviewer assumed that the method was validated in the first trial (pp. 12, 18-19).

Table 2. Initial Validation Method Recoveries for Methiocarb, Methiocarb Sulfoxide and Methiocarb Sulfone in Surface Water^{1,2}

Analyte	Fortification Level (ppb)	Number of Tests	Recovery Range (%)	Mean Recovery (%)	Standard Deviation (%)	Relative Standard Deviation (%)
Quantitation ion						
Methiocarb	0.1 (LOQ)	5	84-99	91	6	6
	1	5	55-97	75	15	20
Methiocarb sulfoxide	0.1 (LOQ)	5 ³	58-125	103	26	25
	1	5	71-110	88	14	16
Methiocarb sulfone	0.1 (LOQ)	5 ³	23-108	81	34	42
	1	5	50-83	70	14	20
Confirmation ion						
Methiocarb	0.1 (LOQ)	5	81-97	90	6	7
	1	5	55-97	75	15	20
Methiocarb sulfoxide	0.1 (LOQ)	5 ³	56-118	99	25	25
	1	5	74-109	90	13	15
Methiocarb sulfone	0.1 (LOQ)	5 ³	29-107	83	31	38
	1	5	50-84	71	14	20

Data (uncorrected recovery results, Appendix D, pp. 74-76) were obtained from Table I, pp. 32-33; Appendix D, pp. 75-76 of MRID 49502503; and DER Attachment 2.

- The surface water was collected from Richmond, California (Inventory No. 2465W-004; source not further specified; p. 18). The water matrix was characterized by Agvise Laboratories, Northwood, North Dakota (p. 19; Appendix C, p. 73).
- Two parent-daughter ion transitions (quantitative = Q, confirmatory = C) were monitored: m/z 226 \rightarrow 169 (Q) and m/z 226 \rightarrow 121 (C) for methiocarb; m/z 242 \rightarrow 185 (Q) and m/z 242 \rightarrow 170 (C) for methiocarb sulfoxide; and m/z 258 \rightarrow 107 (Q) and m/z 258 \rightarrow 202 (C) for methiocarb sulfone (p. 24; Appendix D, pp. 74-76).
- These results include the outlier the study author excluded based on Dixon's Q test at the 99% confidence level (Table I, pp. 32-33; Appendix D, pp. 75-76). Excluding the outliers at the LOQ ($n = 4$), mean \pm standard deviation (relative standard deviation) values for methiocarb sulfoxide were $114 \pm 8\%$ (7%) for Q ion and $110 \pm 7\%$ (6%) for C ion, and for methiocarb sulfone were $96 \pm 13\%$ (14%) for Q ion and $97 \pm 9\%$ (10%) for C ion.

Table 3. Independent Validation Method Recoveries for Methiocarb sulfoxide and Methiocarb sulfoxide Sulfone in Surface (Lake) Water¹

Analyte	Fortification Level (ppb)	Number of Tests	Recovery Range (%)	Mean Recovery (%)	Standard Deviation (%)	Relative Standard Deviation (%)
Quantitation ion						
Methiocarb	0.1 (LOQ)	5	87.6-93.1	90.2	2.61	2.9
	1	5	85.5-90.4	88.3	1.92	2.2
Methiocarb sulfoxide	0.1 (LOQ)	5	91.3-99.4	94.4	3.04	3.2
	1	5	87.9-94.8	90.8	2.87	3.2
Methiocarb sulfone	0.1 (LOQ)	5	78.7-89.3	85.5	4.24	5.0
	1	5	85.1-89.2	87.5	2.08	2.4
Confirmation ion						
Methiocarb	0.1 (LOQ)	5	88.3-92.4	90.5	1.81	2.0
	1	5	85.1-92.0	88.0	2.66	3.0
Methiocarb sulfoxide	0.1 (LOQ)	5	91.7-98.2	94.6	2.58	2.7
	1	5	88.1-93.8	90.1	2.51	2.8
Methiocarb sulfone	0.1 (LOQ)	5	78.4-89.7	85.7	4.70	5.5
	1	5	85.3-91.1	87.8	2.46	2.8

Data (uncorrected recovery results, pp. 16-18) were obtained from Tables 2-7, pp. 22-27 of MRID 49519606.

1 The surface water was collected from Tuckahoe Lake in Tuckahoe State Park, Ridgely, Maryland (Inventory No. 2465W-004; p. 13). The water matrix was characterized by Agvise Laboratories, Northwood, North Dakota (Appendix III, p. 152).

2 Two parent-daughter ion transitions (quantitative = Q, confirmatory = C) were monitored: m/z 226 → 169 (Q) and m/z 226 → 121 (C) for methiocarb; m/z 242 → 185 (Q) and m/z 242 → 170 (C) for methiocarb sulfoxide; and m/z 258 → 107 (Q) and m/z 258 → 201 (C) for methiocarb sulfone (p. 16).

III. Method Characteristics

The LOQ and LOD for all analytes were reported in the ECM as 0.1 ppb and 0.02 ppb, respectively (pp. 25, 30 of MRID 49502503). The LOQ represented 10 ng/mL in solution, and the LOD was 20% of the LOQ and represented 2 ng/mL in solution. The LOQ was justified by the acceptable linearity and recovery in the validation study; the LOD was justified by the good sensitivity and linearity in the calibration solution analysis. In the ILV, only the LOQ (0.100 µg/L) was reported; the LOD was not reported (p. 13 of MRID 49519606). No calculations or comparisons to noise level were reported in the ECM or ILV.

Table 4. Method Characteristics

		Methiocarb	Methiocarb sulfoxide	Methiocarb sulfone
Limit of Quantitation (LOQ)		0.1 ppb (0.1 µg/L)		
Limit of Detection (LOD)		0.02 ppb (0.02 µg/L)		
Linearity (calibration curve r^2 and concentration range)	ECM ¹	$r^2 = 0.9996$ (Q) $r^2 = 0.9997$ (C)	$r^2 = 0.9997$ (Q & C)	$r^2 = 0.9995$ (Q) $r^2 = 0.9990$ (C)
	ILV ²	$r^2 = 0.9990$ (Q) $r^2 = 0.9991$ (C)	$r^2 = 0.9981$ (Q) $r^2 = 0.9980$ (C)	$r^2 = 0.9979$ (Q) $r^2 = 0.9965$ (C)
	Concentration range	(2.00-100 ng/mL)		
Repeatable	ECM	Yes at LOQ and 10×LOQ	No at LOQ (RSD of 25% for Q and C ions). Yes at 10×LOQ.	No at LOQ (RSD of 42% for Q ion and 38% for C ion). Yes at 10×LOQ.
		[surface water]		
	ILV	Yes at LOQ and 10×LOQ. [surface (lake) water]		
Reproducible	ILV	Yes at LOQ and 10×LOQ.		
Specific	ECM	Yes, matrix interferences at analyte retention times were <LOD.	Yes, matrix interferences at analyte retention times were <LOD; however, peak integration at 10×LOQ appeared to be above the baseline.	
	ILV		Yes, matrix interferences at analyte retention times were <LOD; however, some minor baseline noise interfered with integration.	

Data were obtained from pp. 18-19, 25, 30; Table I, pp. 32-33; Figures 2-3, pp. 36-41; Figures 7-9, pp. 48-50; Figures 13-15, pp. 54-62; Appendix C, p. 73 of MRID 49502503; and pp. 13-15; Tables 2-7, pp. 22-27; Figures 1-36, pp. 28-63; Appendix III, p. 152 of MRID 49519606; and DER Attachment 2.

- 1 Solvent-based standards were used. ECM r^2 values are reviewer-generated from reported r values of 0.999523597038 to 0.999864718554 for the quantitative and confirmatory ions of methiocarb, methiocarb sulfoxide and methiocarb sulfone (Figures 7-9, pp. 48-50 of MRID 49502503; DER Attachment 2).
- 2 Matrix-matched standards were used. ILV r^2 values are reviewer-generated from reported r values of 0.9983233 to 0.9991672 for the quantitative and confirmatory ions of methiocarb, methiocarb sulfoxide and methiocarb sulfone (Figures 1-3, pp. 28-30; Figures 19-21, pp. 46-48 of MRID 49519606; DER Attachment 2).

IV. Method Deficiencies and Reviewer's Comments

1. The determinations of the LOQ and LOD in the ECM and ILV were not based on scientifically acceptable procedures as defined in 40 CFR Part 136. The LOQ and LOD were not adequately supported by calculations or comparison to background levels. The LOQ was justified by the acceptable linearity and recovery in the validation study; the LOD was justified by the good sensitivity and linearity in the calibration solution analysis. In the ILV, the LOQ was reported from the ECM, and the LOD was not reported.

Detection limits should not be based on the arbitrarily selected lowest concentration in the spiked samples. Additionally, the lowest toxicological level of concern in water was not reported. An LOQ above toxicological levels of concern results in an unacceptable method classification

2. In the ECM, method recoveries at the LOQ ($n = 5$) for methiocarb sulfoxide (RSDs of 25% for both quantitation and confirmation ions) and methiocarb sulfone (RSDs of 42% and 38% for quantitation and confirmation ions, respectively) did not meet OCSPP Guideline 850.6100 criteria for precision and accuracy [mean recoveries for replicates at each spiking level between 70% and 120% and relative standard deviations (RSD) $\leq 20\%$; DER Attachment 2].

The study author excluded method recoveries at the LOQ as outliers from the statistics based on Dixon's Q test at the 99% confidence level: 58% and 56% for methiocarb sulfoxide and 23% and 29% for methiocarb sulfone (quantitative and confirmation ions, respectively Appendix D, pp. 75-76). Excluding the outliers at the LOQ ($n = 4$), mean \pm standard deviation (RSD) values for methiocarb sulfoxide were $114 \pm 8\%$ (7%) for Q ion and $110 \pm 7\%$ (6%) for C ion, and for methiocarb sulfone were $96 \pm 13\%$ (14%) for Q ion and $97 \pm 9\%$ (10%) for C ion (Table I, pp. 32-33).

3. In representative ECM chromatograms of methiocarb sulfone, peak integration at $10 \times \text{LOQ}$ appeared to be above the baseline in the quantitation and confirmation ions (Figure 14c, p. 59 of MRID 49502503). This irregular integration was not observed in the LOQ chromatograms (Figure 13c, p. 56), but was observed to some degree in the LOD chromatograms (Figure 15c, p. 62). In representative ILV chromatograms, some minor baseline noise interfered with integration (more notable in the confirmation ion; Figure 17, p. 44; Figure 35, p. 62 of MRID 49519606). Overall, matrix interferences at analyte retention times were $< \text{LOD}$ in the ECM and ILV.
4. The ILV did not include a reagent blank.
5. Modifications to the ECM by the ILV included: 1) different, but comparable LC/MS/MS equipment; and 2) the use of m/z 242 \rightarrow 185 (Q) and m/z 242 \rightarrow 170 (C) as the monitored ion transitions for methiocarb sulfoxide (pp. 15-16; Table 1, p. 21 of MRID 49519606). None of these modifications were considered significant.

6. The ILV study authors noted the following problem which was encountered: m/z 201 was determined to be the dominant structural isomer of methiocarb sulfone for ion identification, instead of m/z 202 which was reported by the ECM (Appendix V, p. 161 of MRID 49519606). This modification was not considered significant.
7. The ECM study author noted that calibration solutions should be freshly prepared for analysis since methiocarb sulfone is unstable (p. 21 of MRID 49502503). The ILV study authors concurred with this critical step (Appendix V, p. 162 of MRID 49519606).

The ECM study author also noted that due to the instability of methiocarb sulfone, it is recommended that the sample be analyzed on the same day as it is prepared (p. 22 of MRID 49502503).

The ECM study author assessed matrix effects (pp. 27-28; Table II, p. 34 of MRID 49502503). No significant matrix effects were found, so solvent-based calibrants were used.

8. The communications between the ILV study personnel and the ECM study personnel were reported in the ILV (Appendix V, p. 162 of MRID 49519606).
9. In the ILV, it was reported that that one set of twelve samples required 1.5 calendar days to complete, including LC/MS/MS analysis (Appendix V, p. 162 of MRID 49502506). It was reported in the ECM that two subsample sets of eight samples (sixteen samples total) required 24 person hours to complete (pp. 25-26 of MRID 49502503). The preparation and extraction required *ca.* 6 hours per subsample set; subsequent LC/MS analysis and evaluation also required *ca.* 6 hours per subsample set.

V. References

- 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.

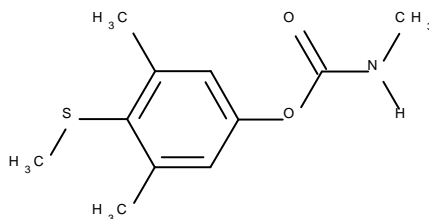
Attachment 1: Chemical Names and Structures**Methiocarb (BAY 37344, Mercaptodimethur)**

IUPAC Name: 4-Methylthio-3,5-xylol methylcarbamate.
3,5-Dimethyl-4-(methylthio)phenyl methylcarbamate.

CAS Name: 3,5-Dimethyl-4-(methylthio)phenyl N-methylcarbamate.

CAS Number: 2032-65-7

SMILES String: CNC(=O)Oc1cc(C)c(SC)c(C)c1

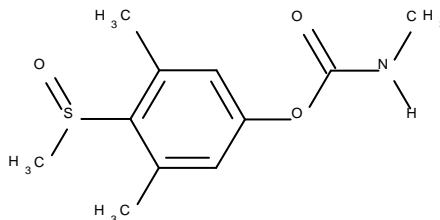
**Methiocarb sulfoxide (MOX)**

IUPAC Name: (3,5-Dimethyl-4-methylsulfinyl-phenyl) N-methylcarbamate.
3,5-Dimethyl-4-(methylsulfinyl)phenyl methylcarbamate.

CAS Name: Phenol, 3,5-Dimethyl-4-(methylsulfinyl)-, methylcarbamate.

CAS Number: 2635-10-1

SMILES String: S(=O)(C)c(c(cc1OC(=O)NC)C)c(c1)C

**Methiocarb sulfone (MON)**

IUPAC Name: (3,5-Dimethyl-4-methylsulfonyl-phenyl) N-methylcarbamate.
3,5-Dimethyl-4-(methylsulfonyl)phenyl methylcarbamate.

CAS Name: Phenol, 3,5-Dimethyl-4-(methylsulfonyl)-, methylcarbamate.

CAS Number: 2179-25-1

SMILES String: S(=O)(=O)(C)c(c(cc1OC(=O)NC)C)c(c1)C

