

US EPA ARCHIVE DOCUMENT

Data Evaluation Report on the hydrolysis of pyrasulfotole (AE 0317309)

PMRA Submission Number 2006-2445

EPA MRID Number 46801705

Data Requirement: PMRA Data Code:
EPA DP Barcode: D328639
OECD Data Point:
EPA Guideline: 161-1

Test material:

Common name: Pyrasulfotole.

Chemical name:

IUPAC name: (5-Hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α -trifluoro-2-mesyl-*p*-tolyl)methanone.

(5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone.

CAS name: (5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-methylsulfonyl]-4(trifluoromethyl)phenyl]methanone.

Methanone, (5-hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl].

CAS No.: 365400-11-9.

Synonyms: AE 0317309; K-1196; K-1267.

Smiles string: FC(c1cc(c(cc1)C(=O)c1c(n(nc1C)C)O)S(=O)(=O)C)(F)F (ISIS v2.3/Universal SMILES).

No EPI Suite, v3.12 SMILES String found as of 6/7/06.

Cc1nn(C)c(O)c1C(=O)c2ccc(C(F)(F)F)cc2S(C)(=O)=O.CS(=O)(=O)c1c(ccc(c1)C(F)(F)F)C(=O)c1c(n(nc1C)C)O.

Primary Reviewer: Dana Worcester
Cambridge Environmental

Signature:
Date: 6/14/06

Secondary Reviewer: Kathleen Ferguson
Cambridge Environmental

Signature:
Date: 6/14/06

QC Manager: Joan Gaidos
Cambridge Environmental

Signature:
Date: 6/14/06

Final Reviewer: Marietta Echeverria
EPA Reviewer

Signature: *Marietta Echeverria*
Date: 11/23/07

Final Reviewer: JD Whall (Officer No. 1268)
PMRA Reviewer

Signature: *J.D. Whall*
Date: 09/18/06 5/16/07

Final Reviewer: Olga Braga
DEH Reviewer

Signature:
Date: 21 Nov 2006

Olga Braga
24/01/2009



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PMRA Submission Number 2006-2445

EPA MRID Number 46801705

Company Code: BCZ
Active Code: PSA
Use Site Category: 13, 14
EPA PC Code: 000692

CITATION: Ripperger, R. 2004. [Pyrazole-3-¹⁴C] AE0317309: hydrolytic degradation. Unpublished study performed and submitted by Bayer CropScience. Research Triangle Park, NC. Bayer Study No.: A9072401; Bayer Report No.: 200578. Experiment started February 5, 2003, and completed March 10, 2003 (p. 6). Final report issued March 22, 2004.

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EXECUTIVE SUMMARY

The hydrolysis of [pyrazole-3-¹⁴C]-labeled (5-hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α -trifluoro-2-mesyl-*p*-tolyl)methanone (pyrasulfotole, AE 0317309, radiochemical purity 98.4%), at 0.14 mg a.i./L, was studied in the dark at $24.9 \pm 0.02^\circ\text{C}$ in sterile aqueous buffered pH 5 (0.01M acetate), pH 7 (0.01M TRIS), and pH 9 (*ca.* 0.009M borate) solutions for 30 days. This experiment was conducted in accordance with USEPA Subdivision N §161-1 guidelines and in compliance with USEPA GLP standards. The test system consisted of amber glass serum vials (30-mL volume) containing treated buffer solution (20 mL) that were sealed with Teflon-lined crimp caps. Duplicate vials of each buffer were collected for analysis at 0, 2, 7, 14, 22, and 30 days posttreatment. Aliquots of the buffers were analyzed directly using LSC and HPLC. Pyrasulfotole was identified by comparison to the HPLC retention time of the test substance and by LC/EIS-MS in the positive mode. There was no attempt to identify transformation products.

During the study, the temperature of the waterbath ranged from 24.1 - 25.0°C and the pHs of the buffer solutions were 4.96-5.06 (pH 5), 6.95-7.03 (pH 7), and 8.93-9.02 (pH 9). The test solutions remained sterile.

Overall recoveries of [¹⁴C]residues averaged $99.8 \pm 0.5\%$ of the applied (range 99.0-100.5%) from the pH 5 buffer solution, $100.1 \pm 0.4\%$ (99.3-100.6%) from the pH 7 solution, and $100.3 \pm 0.3\%$ (99.8-100.7%) from the pH 9 solution. There was no pattern of loss of material over time from any of the buffer solutions.

[¹⁴C]Pyrasulfotole averaged 98.4-100.4% of the applied in the pH 5 solutions and 98.6-100.3% in the pH 7 solution. In the pH 9 solution, [¹⁴C]pyrasulfotole averaged 96.6-98.1% of the applied through 22 days posttreatment and 95.7% at 30 days. Half-lives were not calculated.

No major transformation products were isolated and no minor transformation products were identified in any of the buffer solutions. In the pH 5 and pH 7 buffers, Unknown A (*Rt ca.* 2 minutes) averaged maximums of 1.3-1.5% of the applied. In the pH 9 buffer, Unknowns A, B and C averaged maximums of 0.9%, 3.3%, and 1.4% of the applied, respectively. Volatiles were not measured.

A transformation pathway was not proposed by the study author. A transformation pathway could not be developed because pyrasulfotole was stable to hydrolysis under the conditions of this study.

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RESULTS SYNOPSIS:

pH	Half life	Transformation products	
		Major	Minor
pH 5	Stable.	None.	None.
pH 7	Stable.	None.	None.
pH 9	Stable.	None.	None.

Study Acceptability: This study is classified as **acceptable**. No significant deviations from good scientific practices were noted.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with USEPA Guidelines for Pesticide Registration, Subdivision N §161-1 and Canadian PMRA DACO Number 8.2.3.2 (p. 14). No significant deviations from the objectives of Subdivision N guidelines were noted.

COMPLIANCE: This study was conducted in compliance with USEPA FIFRA GLP Standards (40 CFR Part 160, p. 3). Signed and dated Data Confidentiality, GLP, Quality Assurance, and Certificate of Authenticity statements were provided (pp. 2-5).

A. MATERIALS:

1. Test Material [Pyrazole-3-¹⁴C]pyrasulfotole (p. 14).

Chemical Structure: See DER Attachment 1.

Description: Technical grade (p. 14).

Purity: Radiochemical purity: 98.4% (p. 14).
Batch No.: SEL/1009.
Analytical purity: Not reported.
Specific activity: 54.2 mCi/mMol.
Location of the radiolabel: Labeled on the 3-carbon of the pyrazole ring.

Storage conditions of test chemicals: The test substance, dissolved in acetonitrile, was stored frozen in the dark (p. 14). Storage of reference compounds was not described.

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Physico-chemical properties of pyrasulfotole.

Parameter	Value	Comment
Molecular weight	362.3 g/mol	
Water Solubility (g/L) at 20°C	4.2 at pH 4 69.1 at pH 7 49.0 at pH 9	Very soluble
Vapor Pressure/Volatility	2.7×10^{-7} Pa at 20°C 6.8×10^{-7} Pa at 25°C	Non-volatile
UV Absorption	water $\lambda_{\max} = 264$ 0.1M HCl $\lambda_{\max} = 241$ 0.1M NaOH $\lambda_{\max} = 216$	Not likely to undergo photolysis.
Pka	4.2 ± 0.15	
log K_{ow} at 23°C	0.276 at pH 4 -1.362 at pH 7 -1.58 at pH 9	Not likely to bioaccumulate
Stability of compound at room temperature, if provided		No significant degradation over 12 months at ambient temperatures.

Data obtained from pyrasulfotole chemistry review of Submission 2006-2445.

2. Buffer Solution: Buffer solutions were made with Milli-Q water as follows:

Table 1: Description of buffer solutions.

pH	Type and molarity of buffer	Composition
5	0.01M Acetate	Acetic acid (0.01M in water) was added to 500 mL of 0.01M sodium acetate until a pH of 5 was obtained.
7	0.01M TRIS	ca. 50 mL of 0.1M tris(hydroxymethyl)aminomethane was added to 500 mL of 0.01M HCl to obtain pH 7.
9	ca. 0.009 M Borate	ca 40 mL of 0.1M NaOH was added to 500 mL of 0.01M boric acid to obtain pH 9.

Data obtained from p. 15 of the study report.

B. EXPERIMENTAL CONDITIONS

1. Preliminary Study: A preliminary study (not described) showed that volatiles would not be generated (p. 17). Therefore, a volatile trapping system was not used in this study.

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2. Experimental conditions

Table 2: Experimental parameters

Parameters		Details
Duration of study		30 days.
Test concentrations Nominal: Measured:		0.15 mg/L. 0.14 mg/L.
No. of replications		Two samples were collected at each interval.
Preparation of test medium	Volume used/treatment	37 µL/20 mL.
	Method of sterilization	Vials of untreated solution were sterilized by autoclaving. Sterilization for the stock solution was not reported.
	Co-solvent	Acetonitrile, 0.0009% by volume.
Test apparatus (type/material/volume)		Amber glass serum vials (30-mL volume) containing treated buffer solution (20 mL) were sealed with Teflon-lined crimp caps. The vials were incubated in the dark in a temperature-controlled waterbath at $25.0 \pm 1^\circ\text{C}$. The test apparatus is illustrated in Figure 3, p. 40.
Details of traps for volatile, if any		Volatile traps were not used.
If no traps were used, is the test system closed/open?		Closed.
Is there any indication of the test material adsorbing to the walls of the test apparatus?		None
Experimental conditions Temperature ($^\circ\text{C}$): Lighting: pH ranges:		25 ± 1 . Dark. 4.96-5.06, 6.95-7.03, 8.93-9.02.
Other details, if any		None.

Data were obtained from pp. 16-17, Table 3, p. 27, and Figure 3, p. 40, of the study report.

3. Supplementary Experiments: No supplementary experiments were described.

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4. Sampling:

Table 3: Sampling details.

Criteria	Details
Sampling intervals	0, 2, 7, 14, 22, and 30 days.
Sampling method	Two vials of each treatment were collected at each interval.
Method of collection of CO ₂ and organic volatile compounds	Volatiles were not collected.
Sampling intervals/times for: pH measurement: Sterility check:	At each sampling interval. At each sampling interval.
Sample storage before analysis	Samples were typically analyzed the day of sampling. Otherwise, samples were stored refrigerated for a maximum of 3 days prior to analysis.
Other observation, if any:	None.

Data were obtained from pp. 17, 20 and Table 2, p. 26 of the study report.

C. ANALYTICAL METHODS

Extraction/clean up/concentration methods: Samples were analyzed as collected, without manipulation or modification (p. 17, Figure 5, p. 42.).

Volatile residue determination: Volatiles were not trapped.

Total ¹⁴C measurement: Aliquots (3 x 1 mL) of each sample were analyzed for total [¹⁴C]residues using LSC (p. 17).

Derivatization method, if used: A derivatization method was not employed.

Identification and quantification of parent compound: The samples (3 x 1 mL) were analyzed for pyrasulfotole using HPLC under the following conditions (p. 18): Phenomenex Columbus C8 column (150 x 4.6 mm, 5 Φ m), gradient mobile phase consisting of (A) 0.1% TFA in water and (B) methanol [percent A:B (v:v), 0-2 minutes, 100:0; 23 minutes, 20:80]; flow rate 1.5 mL/minute; with UV (254 nm) and radioactive flow detection. It was reported that reference standards were not used; [¹⁴C]pyrasulfotole was apparently identified by comparison to the HPLC retention time of the test substance (Rt 18.7 minutes; p. 14, Figure 4, p. 41). The HPLC effluent was collected and analyzed using LSC to determine column recoveries averaging 98.5% (p. 21; Figure 5, p. 42).

The identification of pyrasulfotole was confirmed using LC/ESI-MS in the positive mode (p. 18).

Identification and quantification of transformation products: Transformation products were isolated and quantified using HPLC as described above. There was no attempt to identify transformation products because of the relative stability of pyrasulfotole (pp. 14, 22).

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Detection limits (LOD, LOQ) for the parent compound: For LSC, the Limit of Detection was twice background or 0.05-0.09% of the applied depending on sample size (Appendix 2, p. 46). For HPLC, the Limit of Detection of the radiodetector was 530 dpm or a minimum of *ca.* 1.1% of the applied or 1.6 ppb (p. 20). Limits of Quantification were not reported.

Detection limits (LOD, LOQ) for the transformation products: The Limits of Detection were identical to the parent and LOQs were not reported.

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: During the study, the temperature of the waterbath ranged from 24.1-25.0°C (average $24.9 \pm 0.02^\circ\text{C}$) and the pH of the buffer solutions ranged from 4.96-5.06 (pH 5), 6.95-7.03 (pH 7), and 8.93-9.02 (pH 9; p. 21, Tables 3-4, pp. 27-28). The test solutions remained sterile, with the exception of the pH 7, 30-day replicate 2 samples (p. 21). Results from this sample were similar to those of the sterile replicate, so the data were used in the study.

B. MASS BALANCE: Overall recoveries of [^{14}C]residues averaged $99.8 \pm 0.5\%$ of the applied (range 99.0-100.5%) from the pH 5 buffer solution, $100.1 \pm 0.4\%$ (range 99.3-100.6%) from the pH 7 solution, and $100.3 \pm 0.3\%$ (range 99.8-100.7%) from the pH 9 solution (Tables 5-7, pp. 29-31). There was no pattern of loss of material over time from any of the buffer solutions.

Table 4a: Hydrolysis of pyrasulfotole, expressed as percentage of the applied radioactivity (mean \pm s.d., n = 2), at pH 5.

Compound	Sampling times (days)					
	0	2	7	14	22	30
Pyrasulfotole	99.4 ± 0.6	99.7 ± 0.0	98.7 ± 0.1	98.4 ± 1.7	100.1 ± 0.3	100.4 ± 0.0
Unknown A	0.0 ± 0.0	0.0 ± 0.0	1.3 ± 0.3	0.0, 1.8	0.0 ± 0.0	0.0 ± 0.0
Extractables	99.4 ± 0.6	99.7 ± 0.0	100.0 ± 0.1	99.3 ± 0.4	100.1 ± 0.3	100.4 ± 0.0
CO ₂	Volatiles were not collected.					
Volatile organics	Volatiles were not collected.					
Total Recovery	99.4 ± 0.6	99.7 ± 0.0	100.0 ± 0.1	99.3 ± 0.4	100.1 ± 0.3	100.4 ± 0.0

Data obtained from Table 8, p. 32, and Appendix 4, p. 48, of the study report. Means and standard deviations were calculated by the study author.

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Table 4b: Hydrolysis of pyrasulfotole, expressed as percentage of the applied radioactivity (mean \pm s.d., n = 2), at pH 7.

Compound	Sampling times (days)					
	0	2	7	14	22	30
Pyrasulfotole	100.2 \pm 0.6	98.6 \pm 2.1	100.3 \pm 0.5	100.0 \pm 0.4	98.8 \pm 2.4	99.9 \pm 0.7
Unknown A	0.0 \pm 0.0	0.0, 2.6	0.0 \pm 0.0	0.0 \pm 0.0	0.0, 3.0	0.0 \pm 0.0
Extractables	100.2 \pm 0.6	99.9 \pm 0.3	100.3 \pm 0.5	100.0 \pm 0.4	100.3 \pm 0.3	99.9 \pm 0.7
CO ₂	Volatiles were not collected.					
Volatile organics	Volatiles were not collected.					
Total Recovery	100.2 \pm 0.6	99.9 \pm 0.3	100.3 \pm 0.5	100.0 \pm 0.4	100.3 \pm 0.3	99.9 \pm 0.7

Data obtained from Table 9, p. 33, and Appendix 5, p. 49, of the study report. Means and standard deviations were calculated by the study author.

Table 4c: Hydrolysis of pyrasulfotole, expressed as percentage of the applied radioactivity (mean \pm s.d., n = 2), at pH 9.

Compound	Sampling times (days)					
	0	2	7	14	22	30
Pyrasulfotole	97.6 \pm 0.4	98.1 \pm 0.3	96.6 \pm 0.4	97.5 \pm 0.2	96.9 \pm 1.8	95.7 \pm 0.1
Unknown A	0.0 \pm 0.0	0.0 \pm 0.0	0.0 \pm 0.0	0.0 \pm 0.0	0.9 \pm 1.2	0.0 \pm 0.0
Unknown B	2.9 \pm 0.3	2.4 \pm 0.3	3.3 \pm 0.2	2.6 \pm 0.2	2.6 \pm 0.2	3.1 \pm 0.3
Unknown C	0.0 \pm 0.0	0.0 \pm 0.0	0.0 \pm 0.0	0.0 \pm 0.0	0.0 \pm 0.0	1.4 \pm 0.1
Extractables	100.4 \pm 0.1	100.5 \pm 0.0	100.0 \pm 0.2	100.1 \pm 0.3	100.4 \pm 0.4	100.3 \pm 0.1
CO ₂	Volatiles were not collected.					
Volatile organics	Volatiles were not collected.					
Total Recovery	100.4 \pm 0.1	100.5 \pm 0.0	100.0 \pm 0.2	100.1 \pm 0.3	100.4 \pm 0.4	100.3 \pm 0.1

Data obtained from Table 10, p. 34, and Appendix 6, p. 50, of the study report. Means and standard deviations were calculated by the study author.

C. TRANSFORMATION OF PARENT COMPOUND: [¹⁴C]Pyrasulfotole was relatively stable in all three buffer solutions. [¹⁴C]Pyrasulfotole averaged 98.4-100.4% of the applied in the pH 5 solutions and 98.6-100.3% in the pH 7 solution with no pattern of decline (Tables 8-9, pp. 32-33). In the pH 9 solution, [¹⁴C]pyrasulfotole averaged 96.6-98.1% of the applied through 22 days posttreatment and 95.7% at 30 days (Table 10, p. 34).

HALF-LIVES/DT50/DT90: Since [¹⁴C]pyrasulfotole showed no decline in the pH 5 and 7 solutions and declined by <2.5% over 30 days in the pH 9 solution, half-lives were not calculated.

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Half-lives/DT50/DT90

pH	First order linear			DT50	DT90
	Half-life (days)	Regression equation	r ²		
5	Stable.	---	---	---	---
7	Stable.	---	---	---	---
9	Stable.	---	---	---	---

TRANSFORMATION PRODUCTS: No major transformation products were isolated and no minor transformation products were identified in any of the buffer solutions (Tables 8-10, pp. 32-34). In the pH 5 and pH 7 buffers, Unknown A (Rt ca. 2 minutes) averaged maximums of 1.3-1.5% of the applied (Tables 8 and 9, pp. 32-33; Figure 6, p. 43). In the pH 9 buffer, Unknowns A, B and C averaged maximums of 0.9%, 3.3%, and 1.4% of the applied, respectively (Table 10, p. 34). Unknown B (Rt ca. 17.5 minutes) averaged 2.9% of the applied at time 0 and 2.4-3.3% of the applied throughout the study (Figure 6, p. 43).

Table 5: Chemical names and CAS numbers for the transformation products of pyrasulfotole.

Applicants Code Name	CAS Number	Chemical Name	Chemical Formula	Molecular Weight (g/mol)	Smiles String
No transformation products were identified.					

VOLATILIZATION: Volatiles were not measured.

TRANSFORMATION PATHWAY: A transformation pathway was not proposed by the study author. A transformation pathway could not be developed because pyrasulfotole was stable to hydrolysis under the conditions of this study.

D. SUPPLEMENTARY EXPERIMENT-RESULTS: No supplementary experiments were described.

III. STUDY DEFICIENCIES

No significant deviations from good scientific practices or Subdivision N guidelines were noted.

IV. REVIEWERS' COMMENTS

1. The study author reported that the test solutions were analyzed by HPLC using direct injection (Figure 5, p. 42). However, the data tables include rows for organic and aqueous phases or for total extractable residues, with the organic phases entries being "n/a" (Tables 5-10, pp. 29-34). "n/a" was not defined. The reviewer believes that the

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study author was working from a table template and did not remove rows requesting information that was not applicable to this study.

2. Although reference compounds were identified (Figure 1, p. 38), it was stated that "reference standards were not utilized because no significant degradation of the parent compound was observed" (p. 14).
3. The study author reported that the study was restarted due to a failure of the waterbath temperature probe (p. 17). No additional information was provided.
4. The study author did not provide a sample chromatogram showing Unknown C; therefore, the Rt of Unknown C could not be estimated (Figure 6, p. 43).
5. The application rate used in the study was based on an over-spray of surface water at a rate of 75 g/ha assuming a water depth of 5 cm (p. 14).
6. The reviewers agree with the conclusions made by the study author that AE 0317309 did not degrade significantly at pH 5, 7 and 9 buffer solution, no major transformation products were formed in the study, and minor degradates did not exceed 3.3% of the AR.

V. REFERENCES

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 161-1. Hydrolysis studies. Office of Pesticide and Toxic Substances, Washington, DC. EPA 540/9-82-021.
2. U.S. Environmental Protection Agency. 1989. FIFRA Accelerated Reregistration, Phase 3 Technical Guidance. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 540/09-90-078.
3. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis - Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 738-R-93-010.

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Attachment 1: Structures of Parent Compound and Transformation Products

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Pyrasulfotole [AE 0317309; K-1196; K-1267]

IUPAC Name: (5-Hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α -trifluoro-2-mesyl-*p*-tolyl)methanone.

(5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone.

CAS Name: (5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-methylsulfonyl]-4-(trifluoromethyl)phenyl]methanone.

Methanone, (5-hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl].

CAS Number: 365400-11-9.

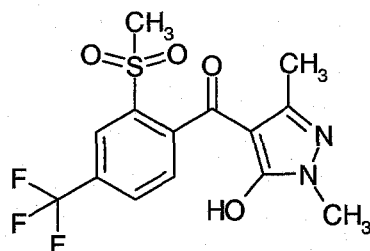
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No EPI Suite, v3.12 SMILES String found as of 6/7/06.

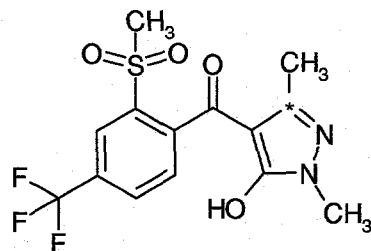
Cc1nn(C)c(O)c1C(=O)c2ccc(C(F)F)cc2S(C)(=O)=O.

CS(=O)(=O)c1c(ccc(c1)C(F)F)C(=O)c1c(n(nc1C)C)O.

Unlabeled



[Pyrazole-3-¹⁴C]pyrasulfotole



¹⁴C = Position of radiolabel.

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Identified Compounds

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Pyrasulfotole [AE 0317309; K-1196; K-1267]

IUPAC Name: (5-Hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α -trifluoro-2-mesyl-*p*-tolyl)methanone.

(5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone.

CAS Name: (5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-methylsulfonyl]-4(trifluoromethyl)phenyl]methanone.

Methanone, (5-hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl].

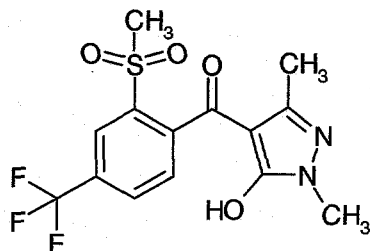
CAS Number: 365400-11-9.

SMILES String: FC(c1cc(c(cc1)C(=O)c1c(n(nc1C)C)O)S(=O)(=O)C)(F)F (ISIS v2.3/Universal SMILES).

No EPI Suite, v3.12 SMILES String found as of 6/7/06.

Cc1nn(C)c(O)c1C(=O)c2ccc(C(F)(F)F)cc2S(C)(=O)=O.

CS(=O)(=O)c1c(ccc(c1)C(F)(F)F)C(=O)c1c(n(nc1C)C)O.



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Unidentified Reference Compounds

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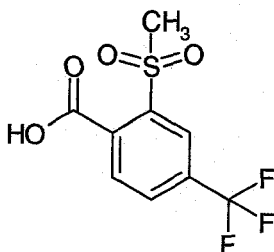
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PMRA Submission Number 2006-2445

EPA MRID Number 46801705

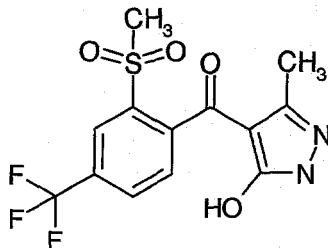
RPA 203328 [AE B197555-benzoic acid; AE B197555; K-1198; K-1367]

IUPAC Name: 2-Mesyl-4-trifluoromethylbenzoic acid.
CAS Name: Benzoic acid, 2-(methylsulfonyl)-4-(trifluoromethyl)-.
CAS Number: 142994-06-7.
SMILES String: O=C(c1ccc(cc1S(=O)(=O)C)C(F)(F)F)O (ISIS v2.3/Universal SMILES).
No EPI Suite, v3.12 SMILES String found as of 6/7/06.
CS(=O)(=O)c1cc(C(F)(F)F)ccc1C(=O)O.
CS(=O)(=O)c1cc(ccc1C(=O)O)C(F)(F)F.



AE 1073910 [AE 0317309 N-Desmethyl; K-1385; K-1197]

IUPAC Name: (5-Hydroxy-3-methyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl]methanone.
CAS Name: Methanone, (5-hydroxy-3-methyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl].
CAS Number: Not reported.
SMILES String: O=C(C2=C(O)NN=C2C)C1=C(S(=O)(C)=O)C=C(C(F)(F)F)C=C1.
CS(=O)(=O)c1cc(ccc1C(=O)c2c([nH]nc2C)O)C(F)(F)F.



Chemical: Pyrasulfotole
MRID: 46801705
PC Code: 000692
Guideline: 161-1

Material Balance

pH 5

Days posttreatment	Recoveries (% Applied)
0	99.0
0	99.8
2	99.7
2	99.7
7	100.1
7	99.9
14	99.6
14	99.0
22	99.9
22	100.3
30	100.5
30	100.4
Average	99.8
SD	0.5

Data obtained from Table 5, p. 29 of the study report.

pH 7

Days posttreatment	Recoveries (% Applied)
0	99.7
0	100.6
2	100.1
2	99.7
7	99.9
7	100.6
14	100.3
14	99.7
22	100.5
22	100.0
30	100.4
30	99.3
Average	100.1
SD	0.4

Data obtained from Table 6, p. 30 of the study report.

pH 9

Days posttreatment	Recoveries (% Applied)
0	100.5
0	100.3
2	100.5
2	100.4
7	100.1
7	99.8
14	99.8
14	100.3
22	100.7
22	100.2
30	100.4
30	100.2
Average	100.3
SD	0.3

Data obtained from Table 7, p. 31 of the study report.