Data Evaluation Repot on the photolysis of pyrasulfotole (AE 0317309) in water

PMRA Submission Number 2006-2445 EPA MRID Number 46801706

Data Requirement: PMRA Data Code: 8.2.3.3.2
EPA DP Barcode: D328639
OECD Data Point: IIA 7.6
EPA Guideline: 161-2

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/QA Manager: Joan Gaidos
Cambridge Environmental
Signature:
Date: 6/14/06

Final Reviewer: Marietta Echeverria
EPA Reviewer
Signature: Marietta Echeverria
Date: 1/23/07

Final Reviewer: JD Whall (Officer No. 1268)
PMRA Reviewer
Signature: J.D. Whall
Date: 5/16/07

Final Reviewer: Olga Braga
DEH Reviewer
Signature:
Date: 24/01/2007

Company Code: BCZ

Data Evaluation Repot on the photolysis of pyrasulfotole (AE 0317309) in water

PMRA Submission Number 2006-2445 EPA MRID Number 46801706

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

CITATION: Ripperger, R.J. and B.N. Meyer. 2005. [^{14}C-UL-Phenyl] and [^{14}C-3-pyrazole] AE0317309: phototransformation in water. Unpublished study performed by Bayer CropScience, Stilwell, KS, and submitted by Bayer CropScience, Research Triangle Park, NC. Study No.: A9082401; Bayer Report No.: 200987. Experiment started July 21, 2003, and completed January 9, 2004 (p. 6). Final report issued March 5, 2005.

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EXECUTIVE SUMMARY

The aqueous phototransformation of [phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-labeled (5-hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α-trifluoro-2-mesyl-*p*-tolyl)methanone (pyrasulfotole, AE 0317309; radiochemical purities 100%), at *ca.* 1 mg a.i./L, was studied in sterile pH 7 buffer (0.01M phosphate) at 25 ± 1°C under continuous irradiation using a UV-filtered xenon arc lamp for 212 hours. The intensity of the lamp was 680 W/m^2; 7.0 hours were reported to be equivalent to 1 solar day in Phoenix, Arizona. This experiment was conducted in accordance with USEPA Subdivision N §161-2 guidelines and in compliance with USEPA GLP standards. The irradiated test system consisted of quartz flat-bottomed vessels (28 x 50 mm, 15 mm deep) containing treated buffer solution (20 mL) that were sealed with ground glass stoppers and placed on a cooling tray within the irradiation apparatus. For the dark controls, amber serum vials with crimp tops were held in a covered circulating waterbath. Volatiles were not collected. Duplicate irradiated samples were collected at 0, 1, 3, 7 and 9 days posttreatment; dark controls were collected at 0, 7 and 9 days. The samples were analyzed for total radioactivity using LSC and for specific [^{14}C]compounds using HPLC. Pyrasulfotole was identified by comparison to the HPLC retention time of the test substance at time 0 and by LC/EIS-MS. There was no attempt to identify transformation products.

The temperatures of the irradiated and dark control samples were maintained at 25.0 ± 0.20°C and 25.0 ± 0.02°C, respectively, and the pH of the solutions ranged from 6.95 to 7.16. The sterility of the solutions was maintained throughout the study.

In the irradiated solutions treated with the phenyl label, overall [^{14}C]residue recoveries averaged 99.8 ± 0.4% (range 98.8-100.2%) of the applied; the corresponding dark controls averaged 99.3 ± 2% (range 95.5-101.4%). In the irradiated solutions treated with the pyrazole label, overall [^{14}C]residue recoveries averaged 100.4 ± 0.3% (range 99.9-100.8%) of the applied; the corresponding dark controls averaged 100.7 ± 1.1% (range 99.9-102.9%). There was no loss of material over time in any sample set.

[^{14}C]Pyrasulfotole (both labels) did not degrade in either the irradiated or dark control solutions. In the irradiated solutions, [^{14}C]pyrasulfotole ranged from an average of 97.7% to 100.7% of the applied with no pattern of decline during the 9-day experiment. In the dark controls, [^{14}C] pyrasulfotole ranged from an average 99.6% to 102.0% of the applied with no pattern of decline. A half-life was not calculated because pyrasulfotole was stable in both the irradiated and dark control solutions.

No major transformation products isolated from either the irradiated or dark control solutions, and no minor transformation products were identified. The only minor transformation product that was isolated (Unknown A) was isolated once, at 4.1% of the applied from one 3-day sample treated with [phenyl-^{14}C]pyrasulfotole. Volatiles were not collected.

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

Results Synopsis

	Half-life (days)	Transformation products	
		Major	Minor
Phenyl label			
Irradiated	Stable.	None	Unknown A.
Dark	Stable.	None.	None.
Pyrazole label			
Irradiated	Stable.	None.	None.
Dark	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 §161-2 (pp. 1, 14).

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 [Phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]pyrasulfotole (p. 14).

Chemical Structure: See DER Attachment 1.

Description: Technical grade (p. 14).

Purity

Phenyl label
Radiochemical purity: 100% (p. 14).
Vial No.: C-938A.
Analytical purity: Not reported.
Specific activity: 28.6 mCi/mMole.
Location of the radiolabel: Uniformly labeled on the phenyl ring.

Pyrazole label
Radiochemical purity: 100% (p. 14).
Vial No.: C-939A.

Analytical purity: Not reported.
Specific activity: 55.3 µCi/mMole.
Location of the radiolabel: On the 3-carbon of the pyrazole moiety.

Storage conditions of test chemicals: The test solutions were stored at <0°C in acetonitrile (p. 14).

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 pyrasulfatole chemistry review of Submission 2006-2445.

2. Buffer Solution

Table 1: Description of buffer solution.

pH	Type and molarity of buffer	Composition
7	0.01M Phosphate	The buffer solution was made by mixing K_2PO_4 in water (1.36 g/L) and adjusting the pH to 7 with 1M KOH.

Data obtained from p. 16 of the study report.

3. Details of light source

Table 2: Artificial light source

Property	Details
Nature of light source	Xenon arc lamp (Atlas).
Emission wavelength spectrum	>290 nm.
Light intensity	680 W/cm^2 between 290 and 800 nm.
Filters used	Suprex (DSET) filter.
Relationship to natural sunlight	The wavelength distribution of the artificial light was comparable to that of natural sunlight. Based on the intensity of the lamp, 7.0 hours of artificial light were reported to be equivalent to 1 day of summer sunlight (June 23, 1988) in New River near Phoenix, Arizona (33.26 N). A comparison of the artificial light to sunlight is presented in Figure 8, p. 47.

Data obtained from pp. 16-17, 51 and Figures 7- 8, pp. 46-47 of the study report.

B. EXPERIMENTAL CONDITIONS:

1. Preliminary Study: A preliminary study (not described) determined that volatiles would not be generated (p. 18). Therefore, a volatile trapping system was not used in this study.

2. Experimental Conditions

Table 3: Experimental Parameters

Parameters		Phenyl	Pyrazole
Duration of the study		9 days.	
Test concentrations (mg a.i./L) Nominal: Measured:		 1 0.99	 1 0.98
Dark controls used (Yes/No)		Yes.	
Replication	Dark	Duplicate samples were collected at each sampling interval.	
	Irradiated	Duplicate samples were collected at each sampling interval.	
Preparation of the test medium:	Volume used/treatment:	315 µL (phenyl) or 540 µL (pyrazole) of test solution were dried, then redissolved in 500 mL of buffer. Aliquots of this solution were transferred to individual sample containers using a syringe with a 0.22 µm sterile filter attached.	
	Method of sterilization:	Glassware was sterilized by autoclaving. The treated buffer solutions were filter-sterilized (0.22 µm) during transfer to the sample containers.	
	Co-solvent (name/concentration), if any:	None, solvent was evaporated and the test material was dissolved in the buffer solution.	

Parameters	Phenyl	Pyrazole
Test apparatus (Type/Material/Volume)	For the irradiated samples, quartz vessels (28 x 50 mm, 15 mm deep, flat-bottomed with an offset neck) containing treated buffer solution (20 mL) were sealed with ground glass stoppers and placed on a cooling tray within the irradiation apparatus. For the dark controls, amber serum vials with crimp tops were held in a covered circulating waterbath. The sample containers used during irradiation are illustrated in Figure 6, p. 45.	
Details of traps for volatile compounds, if any	Volatiles were not collected.	
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; Duration of light/darkness:	 25 ± 1°C. Continuous.	
Other details, if any	None.	

Data obtained from pp. 18-19, Table 1, p. 27, and Figure 6, p. 45 of the study report.

3. Supplementary experiments: No supplementary experiments were described.

4. Sampling:

Table 4: Sampling details

Observations	Details
Sampling intervals	Irradiated: 0, 1, 3, 7 and 9 days. Dark control: 0, 7, and 9 days.
Sampling method	Duplicate samples were collected from each treatment at each sampling interval.
Method of sampling volatile compounds, if any	Volatiles were not collected.
Sampling intervals/times for: Sterility check pH measurement	 At each sampling interval. At each sampling interval.
Sample storage before analysis, if any	Samples were "typically" analyzed on the day of collection, with the maximum storage being 2 days. Samples were stored refrigerated when not in use.
Other observation, if any	None.

Data obtained from p. 19 and Table 2, p. 28 of the study report.

C. ANALYTICAL METHODS:

Extraction/clean up/concentration methods: Samples were analyzed as collected, without manipulation or modification (p. 19, Figure 9, p. 48).

Volatile residue determination: Volatiles were not trapped.

Total ^{14}C measurement: Total [^{14}C]residues were determined by LSC analysis of aliquots (3 x 0.1 mL) of the samples (p. 19, Figure 9, p. 48).

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

Identification and quantification of parent compound: Aliquots (1 x 0.5 or 1.0 mL) of the samples were analyzed for pyrasulfotole using HPLC under the following conditions (pp. 19-20): Phenomenex Columbus C8 column (150 x 4.6 mm, 5 Φm), gradient mobile phase consisting of (A) 0.1% TFA in water and (B) methanol [percent A:B (v:v), 0-2 minutes 100:0; 25-28 minutes 5:95]; flow rate 1.5 mL/minute; and UV (254 nm) and radioactive flow detection. [^{14}C]Pyrasulfotole was identified by comparison to the HPLC retention time of the test substance at time 0 (Rt 18.7-19.4 minutes; p. 15, Figure 2, p. 41). HPLC column recoveries averaged 98.5% (p. 23).

The identification of pyrasulfotole was confirmed using LC/EIS-MS (pp. 21, 24; Figures 3-4, pp. 42-43).

Identification and quantification of transformation products: Transformation products were separated and quantified as described above. No attempt was made to identify transformation products (p. 21).

Detection limits (LOD, LOQ) for the parent: For the HPLC radiodetector, the LOD was 1,000 dpm or 1.14% of the applied (11 ppb; p. 22). For LSC, the LOD was 0.01% of the applied (Appendices 5-6, pp. 54-55). LOQ values were not reported.

Detection limits (LOD, LOQ) for the transformation: LOD and LOQ were the same as reported for the parent.

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: The temperature of the irradiated samples averaged 25.0 ± 0.20°C, ranging from 24.7 to 25.6°C (p. 23, Table 4, p. 30). The temperature of the dark controls averaged 25.0 ± 0.02°C. The pH of the solutions ranged from 6.95 to 7.16 (Table 3, p. 29). The sterility of the solutions was maintained throughout the study.

B. MASS BALANCE: In the irradiated solutions treated with the phenyl label, overall [^{14}C]residue recoveries averaged 99.8 ± 0.4% (range 98.8-100.2%) of the applied; the corresponding dark controls averaged 99.3 ± 2% (range 95.5-101.4%; Table 5, pp. 31-32). In the irradiated solutions treated with the pyrazole label, overall [^{14}C]residue recoveries averaged 100.4 ± 0.3% (range 99.9-100.8%) of the applied; the corresponding dark controls averaged 100.7 ± 1.1% (range 99.9-102.9%). There was no loss of material over time in any sample set.

Table 5a: Phototransformation of [phenyl-^{14}C]pyrasulfotole, expressed as percentage of the applied radioactivity (n = 2), in sterile pH 7 buffer.

Compound		Sampling times (days)				
		0	1	3	7	9
Pyrasulfotole	Irradiated	100.0 ± 0.1	99.9 ± 0.0	97.7 ± 2.6	99.9 ± 0.4	99.5 ± 0.9
	Dark	100.0 ± 0.1	---	---	100.7 ± 1.1	99.6 ± 1.0
Unknown A	Irradiated	0.0 ± 0.0	0.0 ± 0.0	4.1, 0.0	0.0 ± 0.0	0.0 ± 0.0
	Dark	0.0 ± 0.0	---	---	0.0 ± 0.0	0.0 ± 0.0
Total Extractables	Irradiated	100.0 ± 0.1	99.9 ± 0.0	99.7 ± 0.3	99.9 ± 0.4	99.5 ± 0.9
	Dark	100.0 ± 0.1	---	---	100.7 ± 1.1	99.6 ± 1.0
CO_2	Irradiated	Volatiles were not collected.				
	Dark					
Volatile organics	Irradiated	Volatiles were not collected.				
	Dark					
Total recovery	Irradiated	100.0 ± 0.1	99.9 ± 0.0	99.7 ± 0.3	99.9 ± 0.4	99.5 ± 0.9
	Dark	100.0 ± 0.1	---	---	100.7 ± 1.1	99.6 ± 1.0

Data obtained from Table 7, p. 35 and Appendix 8, p. 57 of the study report. Means and standard deviations were calculated by the study authors.

Table 5b: Phototransformation of [pyrazole-3-^{14}C]pyrasulfotole, expressed as percentage of the applied radioactivity (n = 2), in sterile pH 7 buffer.

Compound		Sampling times (days)				
		0	1	3	7	9
Pyrasulfotole	Irradiated	100.0 ± 0.1	100.4 ± 0.3	100.7 ± 0.1	100.6 ± 0.1	100.1 ± 0.2
	Dark	100.0 ± 0.1	---	---	100.2 ± 0.0	102.0 ± 1.2
Total Extractables	Irradiated	100.0 ± 0.1	100.4 ± 0.3	100.7 ± 0.1	100.6 ± 0.1	100.1 ± 0.2
	Dark	100.0 ± 0.1	---	---	100.2 ± 0.0	102.0 ± 1.2
CO_2	Irradiated	Volatiles were not collected.				
	Dark					
Volatile organics	Irradiated	Volatiles were not collected.				
	Dark					
Total recovery	Irradiated	100.0 ± 0.1	100.4 ± 0.3	100.7 ± 0.1	100.6 ± 0.1	100.1 ± 0.2
	Dark	100.0 ± 0.1	---	---	100.2 ± 0.0	102.0 ± 1.2

Data obtained from Table 8, p. 36 and Appendix 9, p. 58 of the study report. Means and standard deviations were calculated by the study authors.

C. TRANSFORMATION OF PARENT COMPOUND: [^{14}C]Pyrasulfotole (both labels) did not degrade in either the irradiated or dark control solutions (Tables 7-8, pp. 35-36). In the irradiated solutions, [^{14}C]pyrasulfotole ranged from an average of 97.7% to 100.7% of the applied with no pattern of decline during the 9-day experiment. In the dark controls, [^{14}C] pyrasulfotole ranged from an average 99.6% to 102.0% of the applied with no pattern of decline.

HALF-LIFE/DT50/DT90: A half-life was not calculated because pyrasulfotole was stable in both the irradiated and dark control solutions. The observed DT50 was >9 days.

Half-lives/DT50/DT90

Treatment	First order linear			DT50 (days)	DT90 (days)
	Half-life (days)	Regression equation	r^2		
Phenyl label					
Irradiated	Stable.			---	---
Dark	Stable.			---	---
Pyrazole label					
Irradiated	Stable.			---	---
Dark	Stable.			---	---

Since pyrasulfotole was stable, the **phototransformation half-life** and **environmental phototransformation half-life** cannot be calculated.

TRANSFORMATION PRODUCTS: No major transformation products were isolated from either the irradiated or dark control solutions (Table 7-8, pp. 35-36). No minor transformation products were identified in either the irradiated or dark control solutions. One minor transformation product (HPLC peak "Unknown A") was isolated once, at 4.1% of the applied from one 3-day sample treated with [phenyl-^{14}C]pyrasulfotole (Appendix 8, p. 57).

Table 6: 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.					

VOLATIZATION: Volatiles were not collected.

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

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

III. STUDY DEFICIENCIES

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

IV. REVIEWERS' COMMENTS

1. AE 0317309 did not degrade in aqueous solution under continuous irradiation. The only degradate observed, at 4.1% of applied, was only found in one replicate at one sampling date (day 3) and thus the possibility that this some type of an artifact cannot be ruled out.

2. The duration of the study is repeatedly defined as 9 days. However, the actual time of irradiation was 212 hours or 8.8 days of continuous irradiation (p. 23).

3. The wavelength distribution of the artificial light was comparable to that of natural sunlight. Based on the intensity of the lamp, 7.0 hours of artificial light were reported to be equivalent to 1 day of summer sunlight (June 23, 1988) in New River near Phoenix, Arizona (33.26 N). Therefore, 212 experimental hours is equivalent to 30.0 environmental days.

4. The study authors stated that "...minor transformation products...comprised a total of ≤4.3% of the applied radioactivity, at any interval. No single metabolite exceed [*sic*] 2.5% of applied radioactivity" (p. 21). However, in Appendices 8 and 9, pyrasulfotole comprises 100% of the recovered radioactivity in all samples at all sampling intervals except once, when Unknown A is 4.1% of the applied in a single sample (2.05% average). It could not be determined what the study authors were referring to when they cited values of 4.3 and 2.5%.

5. Although reference compounds were identified (Figure 1, pp. 39-40), it was stated that "reference standards were not used since limited degradation...was observed" (p. 15).

6. An HPLC chromatogram showing Unknown A was not provided in the study report. The retention time for this peak was not reported, so it was not possible to correlate this peak with results from other studies in this data package.

V. REFERENCES

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 161-2. Photolysis 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.

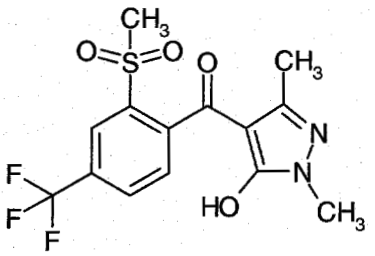
3. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis - Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 738-R-93-010.

Attachment 1: Structures of Parent Compound and Transformation Products

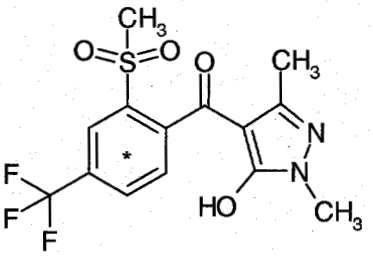
Pyrasulfotole [AE 0317309; K-1196; K-1267]

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.

Unlabeled



[Phenyl-U-^{14}C]pyrasulfotole

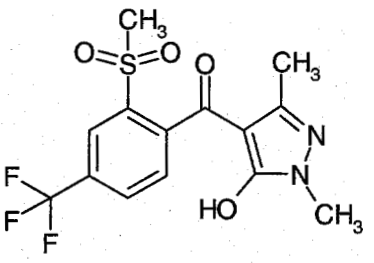


^{14}C = Position of radiolabel.

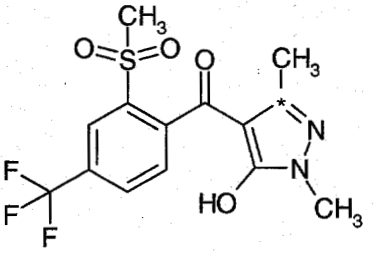
Pyrasulfotole [AE 0317309; K-1196; K-1267]

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.

Unlabeled



[Pyrazole-3-^{14}C]pyrasulfotole

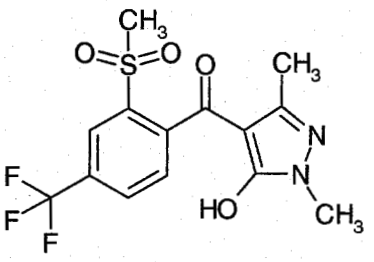


^{14}C = Position of radiolabel.

Identified Compounds

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

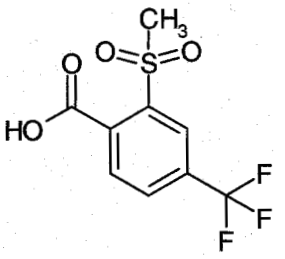
IUPAC Name:	(5-Hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α-trifluoro-2-mesyl-*p*-tolyl)methanone. (5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone.
CAS Name:	(5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-methylsulfonyl)-4(trifluoromethyl)phenyl]methanone. Methanone, (5-hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)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.



Unidentified Reference Compounds

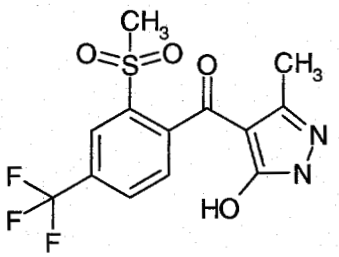
RPA 203328 [AE B197555-benzoic acid; AE B197555; K-1198; K-1367]

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)c1c([nH]nc1C)O)C(F)(F)F.



Chemical: Pyrasulfotole
MRID: 46801706
PC: 000692
Guideline: 161-2

Material Balances

Label: Pyrazole
Irradiated

Days posttreatment	Recoveries (% Applied)
0	99.9
0	100.1
1	100.7
1	100.2
3	100.8
3	100.7
7	100.5
7	100.7
9	100.3
9	100.0
Average	100.4
SD	0.3

Data obtained from Table 6, p. 33 of the study report.

Label: Phenyl
Irradiated

Days posttreatment	Recoveries (% Applied)
0	99.9
0	100.1
1	99.8
1	99.9
3	100.0
3	99.5
7	99.6
7	100.2
9	100.2
9	98.8
Average	99.8
SD	0.4

Data obtained from Table 5, p. 31 of the study report.

Label: Pyrazole
Dark

Days posttreatment	Recoveries (% Applied)
0	99.9
0	100.1
7	100.2
7	100.2
9	101.1
9	102.9
Average	100.7
SD	1.1

Data obtained from Table 6, p. 34 of the study report.

Label: Phenyl
Dark

Days posttreatment	Recoveries (% Applied)
0	99.9
0	100.1
7	101.4
7	99.9
9	95.5
9	98.9
Average	99.3
SD	2.0

Data obtained from Table 5, p. 32 of the study report.