

O,O-Dimethyl phosphorochloridothioate

(O,O-ジメチルホスホロクロリドチオアート)

Experimental Data-1

(B9610-1/4)

Chemical Name	: <u>O,O-Dimethyl phosphorochloridothioate</u>
Synonym	: <u>O,O-Dimethyl thiophosphoryl chloride</u> <u>O,O-Dimethyl chlorothiophosphate</u>
Molecular Weight	: 160.56
Melting Point	: -
Boiling Point	: 68°C(12mmHg)[CHCD]
Flashing Point	: 105°C [Aldrich]
Molecular Formula	: C <sub>2</sub> H <sub>6</sub> ClO <sub>2</sub> PS
Chemical Structure	$  \begin{array}{c}  \text{S} \\     \\  \text{CH}_3\text{O}-\text{P}-\text{Cl} \\    \\  \text{CH}_3\text{O}  \end{array}  $
CAS No.	: 2524-03-0
MITI No.	: (2)-1946
ML No.	:
Specified Chemical Substances	: -
Source of Substance	: Tokyo Kasei Kogyo Co., Ltd.
Lot No.	: FAW01
Purity	: 98.4%
Vehicle	: Acetone

Conc. μ g/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA		TA98		TA1537	
	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
Acetone	( 152 )	( 127 )	( 9 )	( 10 )	( 19 )	( 28 )	( 10 )	( 15 )	( 5 )	( 9 )
	150	158	8	7	20	22	8	21	1	10
	157	138	7	8	17	20	11	16	5	10
1 .22	( 154 )	( 148 )	( 8 )	( 8 )	( 19 )	( 21 )	( 10 )	( 19 )	( 3 )	( 10 )
	178	152	10	2	17	22	8	13	9	7
	137	145	11	10	23	33	9	10	3	7
4 .88	( 158 )	( 149 )	( 11 )	( 6 )	( 20 )	( 28 )	( 9 )	( 12 )	( 6 )	( 7 )
	156	133	7	9	15	20	9	18	5	3
	133	124	5	9	20	29	13	13	5	7
19 .5	( 145 )	( 129 )	( 6 )	( 9 )	( 18 )	( 25 )	( 11 )	( 16 )	( 5 )	( 5 )
	135	144	8	7	21	32	14	17	7	11
	155	162	11	7	32	24	7	24	10	15
78 .1	( 145 )	( 153 )	( 10 )	( 7 )	( 27 )	( 28 )	( 11 )	( 21 )	( 9 )	( 13 )
	137	117 *	14	8 *	29	30	15	15 *	8	9 *
	139	99 *	11	5 *	23	34	15	21 *	2	11 *
313	( 138 )	( 108 *)	( 13 )	( 7 *)	( 26 )	( 32 )	( 15 )	( 18 *)	( 5 )	( 10 *)
	0 *	0 *	0 *	0 *	21 *	37 *	0 *	0 *	0 *	0 *
	0 *	0 *	0 *	0 *	8 *	44 *	0 *	0 *	0 *	0 *
1250	( 0 *)	( 0 *)	( 0 *)	( 0 *)	( 15 *)	( 41 *)	( 0 *)	( 0 *)	( 0 *)	( 0 *)
	0 *	0 *	0 *	0 *	0 *	0 *	0 *	0 *	0 *	0 *
	0 *	0 *	0 *	0 *	0 *	0 *	0 *	0 *	0 *	0 *
5000	( 0 *)	( 0 *)	( 0 *)	( 0 *)	( 0 *)	( 0 *)	( 0 *)	( 0 *)	( 0 *)	( 0 *)
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive Control	AF-2 ( 688 )	2-AA ( 1004 )	NaN <sub>3</sub> ( 290 )	2-AA ( 205 )	AF-2 ( 265 )	2-AA ( 1123 )	AF-2 ( 344 )	2-AA ( 398 )	9-AA ( 781 )	2-AA ( 144 )

\* Growth inhibition was observed.

Mutagenicity in Bacterial Test ; Positive

IARC Evaluation ; not yet cited

Experimental Data-2

(B9610-2/4)

Conc. $\mu$ g/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2 $uvrA$		TA98		TA1537	
Acetone	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
		( 159 )	( 139 )	( 8 )	( 11 )	( 20 )	( 24 )	( 11 )	( 17 )	( 9 )
		129		13				8		9
9 .77		128 ( 129 )		13 ( 13 )				16 ( 12 )		14 ( 12 )
		145		10				15		13
19 .5		135 ( 140 )		16 ( 13 )				21 ( 18 )		11 ( 12 )
	145	126	9	11	25	28	14	26	10	15
39 .1	135 ( 140 )	157 ( 142 )	5 ( 7 )	9 ( 10 )	9 ( 17 )	24 ( 26 )	13 ( 14 )	24 ( 25 )	6 ( 8 )	9 ( 12 )
	144	124	8	6	20	25	15	21	7	13
78 .1	145 ( 145 )	131 ( 128 )	8 ( 8 )	7 ( 7 )	20 ( 20 )	23 ( 24 )	15 ( 15 )	24 ( 23 )	9 ( 8 )	13 ( 13 )
	127	114	14	8	26	30	21	22	5	13
156	143 ( 135 )	142 ( 128 )	6 ( 10 )	5 ( 7 )	15 ( 21 )	40 ( 35 )	16 ( 19 )	25 ( 24 )	5 ( 5 )	11 ( 12 )
	137	105 *	6	8 *	24	33	20	31 *	7	8 *
313	173 ( 155 )	127 * ( 116 *)	10 ( 8 )	9 * ( 9 *)	30 ( 27 )	33 ( 33 )	28 ( 24 )	22 * ( 27 *)	7 ( 7 )	11 * ( 10 *)
	123		7		28	47	22		6	
625	149 ( 136 )		5 ( 6 )		29 ( 29 )	40 ( 44 )	17 ( 20 )		8 ( 7 )	
	0 *		0 *		41 *	40 *	0 *		0 *	
1250	0 * ( 0 *)		0 * ( 0 *)		47 * ( 44 *)	34 * ( 37 *)	0 * ( 0 *)		0 * ( 0 *)	
Judgement	—	—	—	—	—	—	—	—	—	—
Specific Mutagenicity										
Positive Control	AF-2 ( 733 )	2-AA ( 947 )	NaN <sub>3</sub> ( 243 )	2-AA ( 201 )	AF-2 ( 286 )	2-AA ( 1107 )	AF-2 ( 375 )	2-AA ( 388 )	9-AA ( 809 )	2-AA ( 144 )

Experimental Data-3

Conc. μ g/plate	Number of Revertants/plate	
	Base-substitution	Frame-shift
	WP2uvrA	TA98
Acetone	S9-	S9-
	( 24 )	( 18 )
234	25	28
	( 27 )	( 30 )
313	29	28
	( 30 )	( 31 )
469	34	24
	( 32 )	( 24 )
625	25	28
	( 28 )	( 26 )
938	40	0 *
	( 38 )	( 0 *)
1250	39 *	0 *
	( 32 *)	( 0 *)
1880	0 *	
	( 0 *)	
2500	0 *	
	( 0 *)	
Judgement	—	—
Specific Mutagenicity		
Positive Control	AF-2 ( 190 )	AF-2 ( 475 )

Experimental Data-4

(B9610-3/4)

Conc. μ g/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2uvrA/pKM101	
	S9-	S9+	S9-	S9+	S9-	S9+
Acetone	( 338 )	( 390 )	( 335 )	( 329 )	( 48 )	( 67 )
	384	402	356	318	52	86
1 .22	( 383 )	( 404 )	( 341 )	( 326 )	( 51 )	( 81 )
	382	405	325	334	49	75
4 .88	( 363 )	( 396 )	( 355 )	( 367 )	( 69 )	( 76 )
	358	393	382	360	66	72
19 .5	( 372 )	( 431 )	( 365 )	( 369 )	( 66 )	( 97 )
	367	399	328	374	72	79
78 .1	( 432 )	( 489 )	( 388 )	( 394 )	( 76 )	( 149 )
	394	441	373	374	67	100
313	( 536 )	( 500 )	( 466 )	( 340 *)	( 93 )	( 173 )
	412	484	382	393	70	139
1250	( 0 *)	( 0 *)	( 0 *)	( 0 *)	( 0 *)	( 0 *)
	451	493	394	394	82	158
5000	( 0 *)	( 0 *)	( 0 *)	( 0 *)	( 0 *)	( 0 *)
	478	496	465	346 *	92	181
Judgement	—	—	—	—	—	+
Specific Mutagenicity						1050
Positive Control	BLM ( 901 )	2-AA ( 1264 )	PA ( 1703 )	2-AA ( 1310 )	AF-2 ( 1917 )	2-AA ( 1134 )

Experimental Data-5

(B9610-4/4)

Conc. μ g/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2uvrA/pKM101	
Acetone	S9-	S9+	S9-	S9+	S9-	S9+
		( 284 )	( 317 )	( 242 )	( 265 )	( 57 )
9 .77				284 259 ( 272 )		92 92 ( 92 )
19 .5			261 250 ( 256 )	314 249 ( 282 )		85 101 ( 93 )
39 .1	335 335 ( 335 )	352 367 ( 360 )	278 290 ( 284 )	284 309 ( 297 )	72 68 ( 70 )	101 117 ( 109 )
78 .1	390 374 ( 382 )	390 418 ( 404 )	297 347 ( 322 )	311 317 ( 314 )	97 74 ( 86 )	129 141 ( 135 )
156	461 468 ( 465 )	402 407 ( 405 )	214 318 ( 266 )	329 314 ( 322 )	75 81 ( 78 )	150 156 ( 153 )
313	440 471 ( 456 )	444 454 ( 449 )	176 * 151 * ( 164 *)	337 * 314 * ( 326 *)	85 89 ( 87 )	173 * 156 * ( 165 *)
625	0 * 0 * ( 0 *)	179 * 166 * ( 173 *)	0 * 0 * ( 0 *)	0 * 0 * ( 0 *)	29 * 51 * ( 40 *)	
1250	0 * 0 * ( 0 *)	0 * 0 * ( 0 *)	0 * 0 * ( 0 *)	0 * 0 * ( 0 *)	0 * 0 * ( 0 *)	
Judgement	-	-	-	-	-	+
Specific Mutagenicity						272
Positive Control	BLM ( 722 )	2-AA ( 1614 )	PA ( 1684 )	2-AA ( 1395 )	AF-2 ( 1577 )	2-AA ( 950 )