O,O-Diethyl phosphorochloridothioate
(*O,O*-ジエチルホスホロクロリドチオアート)

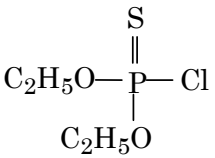
Experimental Data-1

Chemical Name ; *O,O*-Diethyl phosphorochloridothioate

Synonym ; *O,O'*-Diethylthiophosphoryl chloride
O,O-Diethyl chlorothiophospate

Molecular Weight ; 188.61
Melting Point ; −
Boiling Point ; 60℃(2mmHg)[CHCD]
Flashing Point ; >110℃ [Aldrich]
Molecular Formula ; $C_4H_{10}ClO_2PS$

Chemical Structure



CAS No. ; 2524-04-1
MITI No. ; (2)-2939
ML No. ; −
Specified Chemical Substances ; −

Source of Substance; Tokyo Kasei Kogyo Co., Ltd.
Lot No. ; AI01
Purity ; 97.8%

Vehicle ; Acetone

Conc. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2*uvr*A		TA98		TA1537	
	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+
Acetone	(154)	(131)	(9)	(9)	(19)	(27)	(17)	(25)	(6)	(10)
1 .22	134 141 (138)	124 108 (116)	8 6 (7)	5 13 (9)	10 22 (16)	20 21 (21)	24 17 (21)	23 28 (26)	5 3 (4)	6 10 (8)
4 .88	136 119 (128)	138 106 (122)	8 13 (11)	9 8 (9)	34 25 (30)	17 18 (18)	24 17 (21)	28 20 (24)	3 3 (3)	11 15 (13)
19 .5	134 133 (134)	129 128 (129)	6 6 (6)	14 5 (10)	18 18 (18)	38 28 (33)	16 14 (15)	23 26 (25)	8 5 (7)	11 10 (11)
78 .1	148 * 120 * (134 *)	120 133 (127)	5 * 2 * (4 *)	13 10 (12)	21 24 (23)	26 37 (32)	23 11 (17)	26 23 (25)	7 3 (5)	13 15 (14)
313	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)
1250	0 * 0 * (0 *)	0 * 0 * (0 *)	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 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)
Judgement	−	−	−	−	−	−	−	−	−	−
Specific Mutagenicity										
Positive Control	AF-2 (689)	2-AA (1001)	NaN_3 (290)	2-AA (198)	AF-2 (266)	2-AA (1099)	AF-2 (408)	2-AA (392)	9-AA (763)	2-AA (140)

Mutagenicity in Bacterial Test ; Negative

IARC Evaluation ; not yet cited

* Growth inhibitation was observed.

Experimental Data-2

Conc. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2*uvr*A		TA98		TA1537	
	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+
Acetone	(157)	(135)	(9)	(10)	(20)	(25)	(11)	(17)	(8)	(12)
2 .44	146 145 (146)		10 13 (12)							
4 .88	124 150 (137)		7 8 (8)							
9 .77	120 120 (120)	119 124 (122)	8 8 (8)	9 8 (9)	17 22 (20)	15 21 (18)	8 13 (11)	23 17 (20)	6 7 (7)	9 9 (9)
19 .5	131 143 (137)	131 126 (129)	3 8 (6)	9 7 (8)	25 22 (24)	25 28 (27)	10 15 (13)	16 18 (17)	5 6 (6)	10 11 (11)
39 .1	141 130 (136)	139 122 (131)	8 6 (7)	8 3 (6)	20 18 (19)	15 24 (20)	15 15 (15)	20 22 (21)	6 13 (10)	7 10 (9)
78 .1	123 * 105 * (114 *)	129 121 (125)	11 * 3 * (7 *)	3 7 (5)	14 20 (17)	30 30 (30)	13 9 (11)	17 16 (17)	7 6 (7)	20 9 (15)
156		114 * 90 * (102 *)		9 * 3 * (6 *)	0 * 0 * (0 *)	30 28 (29)	0 * 0 * (0 *)	16 * 16 * (16 *)	0 * 0 * (0 *)	7 * 8 * (8 *)
313		0 * 0 * (0 *)		0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)
Judgement	−	−	−	−	−	−	−	−	−	−
Specific Mutagenicity										
Positive Control	AF-2 (725)	2-AA (954)	NaN_3 (235)	2-AA (203)	AF-2 (283)	2-AA (1091)	AF-2 (378)	2-AA (386)	9-AA (787)	2-AA (146)

Experimental Data-3 (B9609-2/3)

Conc. μg/plate	Number of Revertants/plate	
	Base-substitution	
	TA100	TA1535
	S9−	S9−
Acetone	(159)	(8)
2 .44	157 152 (155)	6 13 (10)
4 .88	167 157 (162)	11 7 (9)
9 .77	139 148 (144)	10 9 (10)
19 .5	173 160 (167)	10 3 (7)
39 .1	146 141 (144)	8 7 (8)
78 .1	159 * 138 * (149 *)	7 * 9 * (8 *)
Judgement	−	−
Specific Mutagenicity		
Positive Control	AF-2 (655)	NaN_3 (306)

Experimental Data-4

Conc. μg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2*uvr*A/pKM101	
	S9−	S9+	S9−	S9+	S9−	S9+
Acetone	(333)	(368)	(329)	(332)	(47)	(67)
	326	349	362	342	57	72
	385	358	358	336	66	67
0 .305	(356)	(359)	(360)	(339)	(62)	(70)
	365	353	342	320	52	75
	344	380	342	342	46	77
1 .22	(355)	(367)	(342)	(331)	(49)	(76)
	352	379	350	402	64	83
	382	366	353	318	36	67
4 .88	(367)	(373)	(352)	(360)	(50)	(75)
	341	401	344	293	52	75
	344	376	367	322	52	68
19 .5	(343)	(389)	(356)	(308)	(52)	(72)
	394	407	334	358	30	89
	349	427	329	361	47	66
78 .1	(372)	(417)	(314)	(360)	(39)	(78)
	0 *	0 *	0 *	0 *	0 *	0 *
	0 *	0 *	0 *	0 *	0 *	0 *
313	(0 *)	(0 *)	(0 *)	(0 *)	(0 *)	(0 *)
	0 *	0 *	0 *	0 *	0 *	0 *
	0 *	0 *	0 *	0 *	0 *	0 *
1250	(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 *)
Judgement	−	−	−	−	−	−
Specific Mutagenicity						
Positive Control	BLM (893)	2-AA (1282)	PA (1748)	2-AA (1305)	AF-2 (1956)	2-AA (1139)

Experimental Data-5 (B9609-3/3)

Conc. μg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2*uvr*A/pKM101	
	S9−	S9+	S9−	S9+	S9−	S9+
Acetone	(288)	(316)	(272)	(272)	(55)	(80)
	330	374	310	331	46	75
	318	355	297	312	64	82
9 .77	(324)	(365)	(304)	(322)	(55)	(79)
	307	349	253	318	52	79
	266	379	249	335	66	82
19 .5	(287)	(364)	(251)	(327)	(59)	(81)
	323	349	262	215	57	90
	328	370	228	290	68	78
39 .1	(326)	(360)	(245)	(253)	(63)	(84)
	343	406	236	341	40	69
	272	402	216	271	36	86
78 .1	(308)	(404)	(226)	(306)	(38)	(78)
	0 *	167 *	0 *	176 *	0 *	45 *
	0 *	117 *	0 *	163 *	0 *	29 *
156	(0 *)	(142 *)	(0 *)	(170 *)	(0 *)	(37 *)
	0 *	0 *	0 *	0 *	0 *	0 *
	0 *	0 *	0 *	0 *	0 *	0 *
313	(0 *)	(0 *)	(0 *)	(0 *)	(0 *)	(0 *)
Judgement	−	−	−	−	−	−
Specific Mutagenicity						
Positive Control	BLM (715)	2-AA (1500)	PA (1770)	2-AA (1268)	AF-2 (1591)	2-AA (957)