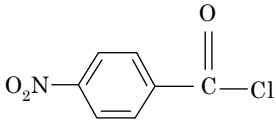


Experimental Data-1

(B9915-1/2)

4-Nitrobenzoyl chloride (4-ニトロベンゾイルクロリド)

Chemical Name	; 4-Nitrobenzoyl chloride	
Synonym	; <u>p</u> -Nitrobenzoyl chloride	
Molecular Weight	; 185.57	
Melting Point	; 75°C	[CHCD]
Boiling Point	; 205°C(105 mmHg)[CHCD]	
Flashing Point	; -	
Molecular Formula	; C <sub>7</sub> H <sub>4</sub> ClNO <sub>3</sub>	
Chemical Structure;		
CAS No.	; 122-04-3	
METI No.	; (3)-1504	
MHLW No.	; -	
Specified Chemical Substances;	-	
Source of Substance;	Tokyo Kasei Kogyo Co., Ltd.	
Lot No.	; GH01	
Purity	; >98%	
Vehicle	; Dehydrated acetone	

Mutagenicity in Bacterial Test: Positive

IARC Evaluation ; not yet cited

Conc. μ g/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA/pKM101		TA98		TA1537	
Acetone	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
		( 125 )	( 124 )	( 10 )	( 7 )	( 64 )	( 85 )	( 16 )	( 26 )	( 9 )
	113	114	6	9	63	93	15	23	10	21
1 .22	143	115	11	9	68	83	17	31	3	13
	( 128 )	( 115 )	( 9 )	( 9 )	( 66 )	( 88 )	( 16 )	( 27 )	( 7 )	( 17 )
	120	139	8	7	68	102	16	31	10	13
4 .88	121	138	3	7	60	94	16	17	9	17
	( 121 )	( 139 )	( 6 )	( 7 )	( 64 )	( 98 )	( 16 )	( 24 )	( 10 )	( 15 )
	162	149	6	10	78	100	14	25	8	22
19 .5	131	143	9	6	75	112	16	32	11	11
	( 147 )	( 146 )	( 8 )	( 8 )	( 77 )	( 106 )	( 15 )	( 29 )	( 10 )	( 17 )
	185	180	9	17	72	79	16	29	7	10
78 .1	197	152	18	15	84	99	9	29	8	15
	( 191 )	( 166 )	( 14 )	( 16 )	( 78 )	( 89 )	( 13 )	( 29 )	( 8 )	( 13 )
	184	171	21	16	93	115	41	28	11	8
313	184	199	28	20	113	97	25	30	11	7
	( 184 )	( 185 )	( 25 )	( 18 )	( 103 )	( 106 )	( 33 )	( 29 )	( 11 )	( 8 )
	0 *	398	0 *	0 *	0 *	128	0 *	40	0 *	5
1250 †	0 *	412	0 *	0 *	0 *	143	0 *	37	0 *	5
	( 0 *)	( 405 )	( 0 *)	( 0 *)	( 0 *)	( 136 )	( 0 *)	( 39 )	( 0 *)	( 5 )
	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 *)
Judgement	-	+	+	+	-	-	+	-	-	-
Specific Mutagenicity		225	47.9	115			54.3			
Positive Control	AF-2	2-AA	NaN <sub>3</sub>	2-AA	AF-2	2-AA	AF-2	2-AA	9-AA	2-AA
	( 703 )	( 1187 )	( 365 )	( 249 )	( 1008 )	( 743 )	( 472 )	( 470 )	( 320 )	( 232 )

\* Growth inhibition was observed.

† Test chemical was precipitated with S9mix.

†† Test chemical was precipitated with and without S9mix.

Experimental Data-2

Conc. μ g/plate	Number of Revertants/plate									
	Base-substitution					Frame-shift				
	TA100		TA1535		WP2uvrA/pKM101	TA98		TA1537		
Acetone	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
	( 120 )	( 115 )	( 10 )	( 9 )	( 72 )	( 98 )	( 11 )	( 27 )	( 7 )	( 13 )
19 .5	136 ( 137 )		11 ( 13 )	13 ( 14 )	61 ( 64 )		21 ( 20 )		7 ( 8 )	
39 .1	128 ( 126 )		9 ( 8 )	13 ( 18 )	68 ( 67 )		33 ( 26 )		8 ( 8 )	
78 .1	163 ( 177 )	169 ( 159 )	10 ( 15 )	13 ( 12 )	84 ( 77 )	76 ( 83 )	31 ( 32 )	31 ( 31 )	5 ( 5 )	11 ( 11 )
156	167 ( 186 )	148 ( 147 )	16 ( 20 )	16 ( 19 )	84 ( 83 )	70 ( 84 )	25 ( 25 )	24 ( 26 )	13 ( 10 )	9 ( 8 )
313	266 ( 247 )	228 ( 221 )	23 ( 31 )	29 ( 25 )	91 ( 100 )	111 ( 108 )	37 ( 37 )	24 ( 27 )	8 ( 7 )	11 ( 9 )
625	0 * ( 0 *)	328 ( 316 )	0 * ( 0 *)	30 ( 31 )	106 ( 103 )	105 ( 98 )	0 * ( 0 *)	37 ( 37 )	6 * ( 8 *)	18 ( 14 )
1250 †	0 * ( 0 *)	483 ( 430 )	0 * ( 0 *)	0 * ( 0 *)	0 * ( 0 *)	145 ( 149 )	0 * ( 0 *)	54 ( 56 )	0 * ( 0 *)	8 ( 7 )
2500 †		0 * ( 0 *)				157 ( 168 )		0 * ( 0 *)		7 ( 5 )
5000 †		0 * ( 0 *)				0 * ( 0 *)		0 * ( 0 *)		0 * ( 0 *)
Judgement	+	+	+	+	-	-	+	+	-	-
Specific Mutagenicity	406	322	67.1	230			384	23.2		
Positive Control	AF-2 ( 728 )	2-AA ( 1402 )	NaN <sub>3</sub> ( 473 )	2-AA ( 239 )	AF-2 ( 883 )	2-AA ( 746 )	AF-2 ( 515 )	2-AA ( 464 )	9-AA ( 390 )	2-AA ( 213 )

\* Growth inhibition was observed.

† Test chemical was precipitated with S9mix.

Experimental Data-3

(B9915-2/2)

Conc. μ g/plate	Number of Revertants/plate		
	Base-substitution	Frame-shift	
	TA100	TA98	
Acetone	S9-	S9-	S9+
	( 128 )	( 19 )	( 30 )
4 .88		24 ( 23 )	
9 .77		13 ( 17 )	
19 .5	163 ( 150 )	31 ( 27 )	
39 .1	186 ( 179 )	52 ( 59 )	
78 .1	202 ( 193 )	62 ( 48 )	22 23 ( 23 )
156	211 ( 227 )	36 ( 36 )	29 31 ( 30 )
313	242 ( 257 )	41 ( 40 )	30 38 ( 34 )
625	0 * ( 0 *)		40 45 ( 43 )
1250	0 * ( 0 *)		61 66 ( 64 )
2500			0 * 0 * ( 0 *)
5000			0 * 0 * ( 0 *)
Judgement	+	+	+
Specific Mutagenicity	412	1020	27.2
Positive Control	AF-2 ( 791 )	AF-2 ( 485 )	2-AA ( 506 )

\* Growth inhibition was observed.