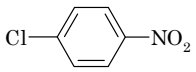
1-Chloro-4-nitrobenzene (1-ｸﾛﾛ-4-ﾆﾄﾛﾍﾞﾝｾﾞﾝ)

Chemical Name ; 1-Chloro-4-nitrobenzene
Synoym ; 4-Chloronitrobenzene
p-Chloronitrobenzene

Molecular Weight ; 157.56
Melting Point ; 83℃[CHCD]
Boiling Point ; 242℃[CHCD]
Flashing Point ; 127℃[Merck]
Molecular Formular; $C_6H_4ClNO_2$

Chemical Structure;



CAS No. ; 100-00-5
METI No. ; (3)-442
MHLW No. ; —
Specified Chemical Substances; Group 2

Source of Substance; Tokyo Kasei Kogyo Co., Ltd.
Lot No. ; GF01
Purity ; >99%

Vehicle ; DMSO

Mutagenicity in Bacterial Test; Positive

IARC Evaluation ; Group 3

Conc. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2*uvrA*/pKM101		TA98		TA1537	
	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+
DMSO	(113)	(115)	(13)	(13)	(78)	(109)	(17)	(24)	(8)	(10)
	127	115	16	17	85	100	22	26	6	9
	126	116	22	18	94	108	8	17	6	9
1 .22	(127)	(116)	(19)	(18)	(90)	(104)	(15)	(22)	(6)	(9)
	111	143	9	21	74	129	9	20	2	8
	87	109	17	15	79	123	14	13	5	3
4 .88	(99)	(126)	(13)	(18)	(77)	(126)	(12)	(17)	(4)	(6)
	115	148	22	13	93	91	18	23	5	5
	145	150	18	13	71	119	14	34	2	6
19 .5	(130)	(149)	(20)	(13)	(82)	(105)	(16)	(29)	(4)	(6)
	137	146	15	11	105	120	18	29	10	6
	111	173	14	11	75	87	15	22	10	6
78 .1	(124)	(160)	(15)	(11)	(90)	(104)	(17)	(26)	(10)	(6)
	121	215	13	15	82	117	28	24	7	6
	129	201	10	18	75	85	21	29	3	10
313	(125)	(208)	(12)	(17)	(79)	(101)	(25)	(27)	(5)	(8)
	99 *	208 *	7 *	20 *	72	96	21	15	6	5
	87 *	212 *	5 *	23 *	78	104	15	21	1	9
1250	(93 *)	(210 *)	(6 *)	(22 *)	(75)	(100)	(18)	(18)	(4)	(7)
	2 *	0 *	0 *	0 *	23	43	0 *	0 *	0 *	0 *
	1 *	0 *	0 *	0 *	33	61	0 *	0 *	0 *	0 *
5000	(2 *)	(0 *)	(0 *)	(0 *)	(28)	(52)	(0 *)	(0 *)	(0 *)	(0 *)
Judgement	—	—	—	—	—	—	—	—	—	—
Specific Mutagenicity										
Positive Control	AF-2 (720)	2-AA (1332)	NaN_3 (450)	2-AA (260)	AF-2 (1135)	2-AA (967)	AF-2 (537)	2-AA (550)	9-AA (404)	2-AA (190)

* Growth inhibition was observed.

Conc. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2*uvrA*/pKM101		TA98		TA1537	
	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+
DMSO	(104)	(114)	(14)	(11)	(71)	(107)	(17)	(23)	(10)	(11)
19 .5		167 160 (164)		13 13 (13)	( )	( )	( )	( )	( )	( )
39 .1	113 142 (128)	163 184 (174)	10 13 (12)	13 16 (15)	( )	( )	( )	( )	( )	( )
78 .1	116 102 (109)	159 164 (162)	16 14 (15)	16 17 (17)	( )	( )	( )	( )	( )	( )
156	127 121 (124)	199 178 (189)	15 15 (15)	18 17 (18)	72 81 (77)	93 91 (92)	13 15 (14)	20 21 (21)	8 5 (7)	6 14 (10)
313	133 137 (135)	185 230 (208)	11 9 (10)	8 14 (11)	75 62 (69)	105 101 (103)	18 23 (21)	18 25 (22)	8 2 (5)	9 5 (7)
625	115 * 123 * (119 *)	219 202 (211)	7 * 3 * (5 *)	16 18 (17)	68 66 (67)	106 86 (96)	7 21 (14)	17 30 (24)	3 2 (3)	5 3 (4)
1250	114 * 112 * (113 *)	211 * 219 * (215 *)	13 * 14 * (14 *)	14 * 18 * (16 *)	70 74 (72)	114 101 (108)	11 11 (11)	24 28 (26)	3 2 (3)	3 5 (4)
2500	( )	194 * 172 * (183 *)	( )	18 * 23 * (21 *)	62 41 (52)	90 106 (98)	8 11 (10)	22 20 (21)	6 * 1 * (4 *)	1 5 (3)
5000	( )	( )	( )	( )	28 36 (32)	34 45 (40)	3 * 2 * (3 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)
Judgement	−	−	−	−	−	−	−	−	−	−
Specific Mutagenicity										
Positive Control	AF-2 (706)	2-AA (1267)	NaN_3 (362)	2-AA (223)	AF-2 (1335)	2-AA (1014)	AF-2 (472)	2-AA (451)	9-AA (513)	2-AA (195)

* Growth inhibition was observed.

Experimental Data-3

Conc. μg/plate	Number of Revertants/plate	
	Base-substitution	
	TA100	
	S9−	S9+
DMSO	(117)	(113)
39 .1	119 133 (126)	148 123 (136)
78 .1	124 133 (129)	121 142 (132)
156	129 129 (129)	171 143 (157)
313	130 127 (129)	193 191 (192)
625	150 108 (129)	192 188 (190)
1250	106 120 (113)	227 234 (231)
2500	105 102 (104)	172 187 (180)
5000	0 * 0 * (0 *)	0 * 0 * (0 *)
Judgement	−	+
Specific Mutagenicity		94.4
Positive Control	AF-2 (637)	2-AA (1883)

* Growth inhibition was observed.

Experimental Data-4 (B0005-3/3)

Conc. μg/plate	Number of Revertants/plate	
	Base-substitution	
	TA100	
	S9−	S9+
DMSO	(105)	(113)
156	108 122 (115)	( )
313	137 121 (129)	( )
500	( )	193 200 (197)
625	104 124 (114)	( )
1000	( )	234 301 (268)
1250	113 120 (117)	( )
1500	( )	233 246 (240)
2000	( )	214 228 (221)
2500	83 69 (76)	209 158 (184)
5000	0 * 0 * (0 *)	( )
Judgement	−	+
Specific Mutagenicity		155
Positive Control	AF-2 (480)	2-AA (1293)

* Growth inhibition was observed.