Allyl chloride(アリルクロリド)

Chemical Name ; Allyl chloride
Synoym ; 塩化アリル
3-Chloro-1-propene

Molecular Weight ; 76.53
Melting Point ; -134.5℃ [CHCD]
Boiling Point ; 45 ℃ [CHCD]
Flashing Point ; -31 ℃(c.c.)[Merck]
Molecular Formular; C_3H_5Cl

Chemical Structure;

$CH_2{=}CHCH_2Cl$

CAS No. ; 107-05-1
METI No. ; (2)-123
MHLW No. ; −
Specified Chemical Substances; −

Source of Substance; Tokyo Kasei Kogyo Co., Ltd.
Lot No. ; FGG01
Purity ; >98%

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	(111)	(111)	(10)	(10)	(63)	(102)	(17)	(21)	(9)	(12)
	108	112	16	8	94	99	16	26	6	10
	112	100	11	7	51	102	10	23	10	8
1 .22	(110)	(106)	(14)	(8)	(73)	(101)	(13)	(25)	(8)	(9)
	122	136	9	14	59	104	24	13	6	15
	133	124	11	6	57	90	14	30	11	16
4 .88	(128)	(130)	(10)	(10)	(58)	(97)	(19)	(22)	(9)	(16)
	87	99	8	9	56	108	20	16	10	9
	92	87	6	11	54	120	9	23	15	24
19 .5	(90)	(93)	(7)	(10)	(55)	(114)	(15)	(20)	(13)	(17)
	97	111	13	9	51	120	15	17	9	10
	107	130	10	3	55	93	23	26	6	14
78 .1	(102)	(121)	(12)	(6)	(53)	(107)	(19)	(22)	(8)	(12)
	102	139	8	6	61	99	14	30	6	25
	130	123	13	8	56	122	7	23	7	9
313	(116)	(131)	(11)	(7)	(59)	(111)	(11)	(27)	(7)	(17)
	159	156	13	14	67	158	22	21	5	20
	178	152	14	9	70	135	25	22	8	8
1250	(169)	(154)	(14)	(12)	(69)	(147)	(24)	(22)	(7)	(14)
	183 *	135 *	36 *	14	186	269	13 *	15 *	8 *	8 *
	198 *	148 *	32 *	11	169	288	17 *	18 *	7 *	7 *
5000	(191 *)	(142 *)	(34 *)	(13)	(178)	(279)	(15 *)	(17 *)	(8 *)	(8 *)
Judgement	−	−	+	−	+	+	−	−	−	−
Specific Mutagenicity			4.8		23	35.4				
Positive Control	AF-2 (623)	2-AA (1485)	NaN_3 (396)	2-AA (258)	AF-2 (831)	2-AA (1017)	AF-2 (528)	2-AA (510)	9-AA (326)	2-AA (203)

* 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	(106)	(109)	(13)	(7)	(72)	(94)	(21)	(25)	(10)	(13)
	137	114	6	8	77	135	21	24	9	8
	104	104	7	8	67	108	21	29	8	9
156	(121)	(109)	(7)	(8)	(72)	(122)	(21)	(27)	(9)	(9)
	82	119	8	7	76	141	15	16	15	6
	133	124	14	7	67	120	23	22	9	11
313	(108)	(122)	(11)	(7)	(72)	(131)	(19)	(19)	(12)	(9)
	141	139	13	8	86	127	26	37	9	7
	141	115	16	8	76	135	22	25	3	14
625	(141)	(127)	(15)	(8)	(81)	(131)	(24)	(31)	(6)	(11)
	145	153	8	10	79	141	23	24	8	11
	171	128	11	6	84	150	24	18	10	6
1250	(158)	(141)	(10)	(8)	(82)	(146)	(24)	(21)	(9)	(9)
	202	152	34	16	123	162	45	29	7	11
	206	119	36	16	105	171	40	30	10	9
2500	(204)	(136)	(35)	(16)	(114)	(167)	(43)	(30)	(9)	(10)
	425 *	218 *	64 *	14	171	209	15 *	31 *	7 *	8 *
	427 *	204 *	74 *	20	151	233	15 *	29 *	3 *	9 *
5000	(426 *)	(211 *)	(69 *)	(17)	(161)	(221)	(15 *)	(30 *)	(5 *)	(9 *)
Judgement	+	−	+	+	+	+	+	−	−	−
Specific Mutagenicity	64		11.2	3.6	17.8	25.4	8.8			
Positive Control	AF-2 (635)	2-AA (1201)	NaN_3 (385)	2-AA (252)	AF-2 (813)	2-AA (1388)	AF-2 (544)	2-AA (435)	9-AA (388)	2-AA (221)

* Growth inhibition was observed.

Conc. μg/plate	Number of Revertants/plate					
	Base-substitution					Frame-shift
	TA100	TA1535		WP2*uvrA*/pKM101		TA98
	S9−	S9−	S9+	S9−	S9+	S9−
DMSO	(120)	(10)	(11)	(65)	(98)	(21)
	131	11	14	67	97	18
	124	16	9	63	115	29
156	(128)	(14)	(12)	(65)	(106)	(24)
	127	16	10	71	105	21
	142	15	10	76	133	28
313	(135)	(16)	(10)	(74)	(119)	(25)
	181	16	13	72	136	33
	149	8	7	71	150	24
625	(165)	(12)	(10)	(72)	(143)	(29)
	192	29	15	89	143	36
	192	15	9	93	142	30
1250	(192)	(22)	(12)	(91)	(143)	(33)
	309	36	7	117	169	31 *
	279	28	18	113	194	44 *
2500	(294)	(32)	(13)	(115)	(182)	(38 *)
	432	24 *	13	209	268	0 *
	419	40 *	22	197	301	0 *
5000	(426)	(32 *)	(18)	(203)	(285)	(0 *)
Judgement	+	+	−	+	+	−
Specific Mutagenicity	69.6	9.6		27.6	37.4	
Positive Control	AF-2 (665)	NaN_3 (397)	2-AA (272)	AF-2 (1458)	2-AA (1057)	AF-2 (419)

* Growth inhibition was observed.