3-Chloropropionic acid (3-ｸﾛﾛﾌﾟﾛﾋﾟｵﾝ酸)

Chemical Name ; 3-Chloropropionic acid
Synoym ; β-Chloropropionic acid

Molecular Weight ; 108.52
Melting Point ; 41、61℃ [CHCD]
Boiling Point ; 204℃(decomposition)[CHCD]
Flashing Point ; >106℃ [CHCD]
Molecular Formular; $C_3H_5ClO_2$

Chemical Structure;

$ClCH_2CH_2COOH$

CAS No. ; 107-94-8
METI No. ; (2)-1157
MHLW No. ; －
Specified Chemical Substances;－

Source of Substance; Tokyo Kasei Kogyo Co., Ltd.
Lot No. ; FIA01
Purity ; >98%

Vehicle ; H_2O

Mutagenicity in Bacterial Test; Positive

IARC Evaluation ; not yet cited

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＋
H_2O	(120)	(136)	(14)	(14)	(70)	(110)	(17)	(22)	(4)	(13)
	123	121	28	20	71	94	14	25	10	14
	128	124	22	24	76	133	17	15	7	16
1 .22	(126)	(123)	(25)	(22)	(74)	(114)	(16)	(20)	(9)	(15)
	136	146	39	44	69	114	23	25	5	7
	158	148	38	44	90	129	25	24	8	8
4 .88	(147)	(147)	(39)	(44)	(80)	(122)	(24)	(25)	(7)	(8)
	192	236	134	146	82	119	16	16	13	6
	183	223	101	163	78	129	16	23	10	10
19 .5	(188)	(230)	(118)	(155)	(80)	(124)	(16)	(20)	(12)	(8)
	449	456	424	476	108	137	16	18	6	8
	444	450	418	504	71	141	22	34	9	3
78 .1	(447)	(453)	(421)	(490)	(90)	(139)	(19)	(26)	(8)	(6)
	957	1148	1117	1240	119	162	21	21	5	13
	1018	1101	1151	1101	101	193	17	32	5	7
313	(988)	(1125)	(1134)	(1171)	(110)	(178)	(19)	(27)	(5)	(10)
	1641	2051	1912	2071	285	383	15	25	7	9
	1716	1980	1862	2121	261	348	13	22	8	11
1250	(1679)	(2016)	(1887)	(2096)	(273)	(366)	(14)	(24)	(8)	(10)
	2404	2582	2458	2632	739	869	24	29	9	11
	2303	3024	2565	2558	807	883	26	23	8	6
5000	(2354)	(2803)	(2512)	(2595)	(773)	(876)	(25)	(26)	(9)	(9)
Judgement	＋	＋	＋	＋	＋	＋	－	－	－	－
Specific Mutagenicity	4190	4060	5330	7230	162	205				
Positive Control	AF-2 (725)	2-AA (1375)	NaN_3 (456)	2-AA (265)	AF-2 (1119)	2-AA (961)	AF-2 (523)	2-AA (550)	9-AA (395)	2-AA (193)

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+
H_2O	(130)	(140)	(12)	(14)	(73)	(96)	(18)	(27)	(7)	(10)
1 .22	( )	( )	36 30 (33)	15 36 (26)	( )	( )	( )	( )	3 5 (4)	( )
2 .44	( )	( )	22 29 (26)	36 40 (38)	( )	( )	( )	( )	7 5 (6)	( )
4 .88	( )	( )	44 41 (43)	66 39 (53)	( )	( )	( )	( )	9 10 (10)	( )
9 .77	( )	( )	59 71 (65)	82 98 (90)	( )	( )	( )	( )	2 7 (5)	( )
19 .5	186 172 (179)	225 223 (224)	127 123 (125)	136 155 (146)	( )	( )	( )	( )	11 2 (7)	( )
39 .1	214 199 (207)	271 265 (268)	284 235 (260)	276 291 (284)	( )	( )	( )	( )	( )	( )
78 .1	330 350 (340)	395 402 (399)	450 445 (448)	470 475 (473)	( )	( )	( )	( )	( )	( )
156	484 496 (490)	614 622 (618)	( )	( )	( )	( )	( )	( )	( )	( )
313	812 786 (799)	1060 1050 (1055)	( )	( )	116 134 (125)	170 150 (160)	16 24 (20)	25 28 (27)	( )	11 5 (8)
625	( )	( )	( )	( )	153 197 (175)	214 216 (215)	16 20 (18)	36 36 (36)	( )	5 3 (4)
1250	( )	( )	( )	( )	271 263 (267)	342 285 (314)	20 20 (20)	41 43 (42)	( )	7 9 (8)
2500	( )	( )	( )	( )	468 521 (495)	514 441 (478)	10 16 (13)	22 18 (20)	( )	10 7 (9)
5000	( )	( )	( )	( )	731 740 (736)	623 650 (637)	36 29 (33)	33 24 (29)	( )	11 6 (9)
Judgement	+	+	+	+	+	+	−	−	−	−
Specific Mutagenicity	2690	3320	17200	9840	169	190				
Positive Control	AF-2 (704)	2-AA (1284)	NaN_3 (376)	2-AA (226)	AF-2 (1468)	2-AA (863)	AF-2 (491)	2-AA (446)	9-AA (514)	2-AA (193)

Experimental Data-3

Conc. μg/plate	Number of Revertants/plate	
	Base-substitution	
	TA1535	
	S9−	S9+
H_2O	(12)	(12)
0 .153	13 18 (16)	16 16 (16)
0 .305	11 18 (15)	13 14 (14)
0 .61	18 11 (15)	14 20 (17)
1 .22	26 26 (26)	17 20 (19)
2 .44	37 22 (30)	31 34 (33)
Judgement	+	+
Specific Mutagenicity	11500	8160
Positive Control	NaN_3 (443)	2-AA (257)

Experimental Data-4

Conc. μg/plate	Number of Revertants/plate
	Frame-shift
	TA1537
	S9−
H_2O	(10)
2 .44	13 8 (11)
4 .88	7 7 (7)
9 .77	6 13 (10)
19 .5	11 8 (10)
39 .1	9 9 (9)
78 .1	13 6 (10)
156	10 15 (13)
313	6 8 (7)
625	7 10 (9)
1250	7 9 (8)
2500	6 10 (8)
5000	6 10 (8)
Judgement	−
Specific Mutagenicity	
Positive Control	9-AA (402)

Experimental Data-5 (B0006-3/3)

Conc. μg/plate	Number of Revertants/plate
	Frame-shift
	TA1537
	S9−
H_2O	(7)
2 .44	8 7 (8)
4 .88	13 5 (9)
9 .77	7 10 (9)
19 .5	10 8 (9)
39 .1	13 6 (10)
78 .1	7 3 (5)
156	10 11 (11)
313	9 5 (7)
625	5 7 (6)
1250	6 10 (8)
2500	3 7 (5)
5000	3 9 (6)
Judgement	−
Specific Mutagenicity	
Positive Control	9-AA (539)