

Butyric acid (酪酸)

Experimental Data-1

(B9603-1/3)

Chemical Name ; <u>Butyric acid</u> Synonym ; <u>Butanoic acid</u> Molecular Weight ; 88.11 Melting Point ; -8 °C[CHCD] Boiling Point ; 163.5°C[CHCD] Flashing Point ; 77 °C[Aldrich] Molecular Formula ; $C_4H_8O_2$ Chemical Structure $CH_3CH_2CH_2COOH$ CAS No. ; 107-92-6 MITI No. ; (2)-608 ML No. ; — Specified Chemical Substances ; — Source of Substance ; Tokyo Kasei Kogyo Co., Ltd. Lot No. ; FAT01 Purity ; 99.0% Vehicle ; H_2O	Conc. μ g/plate	Number of Revertants/plate									
	H_2O	Base-substitution						Frame-shift			
		TA100		TA1535		WP2uvrA		TA98		TA1537	
		S9—	S9+	S9—	S9+	S9—	S9+	S9—	S9+	S9—	S9+
		(148)	(161)	(8)	(10)	(16)	(20)	(15)	(21)	(7)	(9)
		149	169	6	8	17	32	11	22	5	9
	1 .22	162	176	9	11	17	24	21	26	7	8
		(156)	(173)	(8)	(10)	(17)	(28)	(16)	(24)	(6)	(9)
		151	151	8	17	21	25	28	16	6	6
	4 .88	150	197	8	14	18	17	18	26	5	8
		(151)	(174)	(8)	(16)	(20)	(21)	(23)	(21)	(6)	(7)
		180	174	3	9	22	13	20	22	8	6
	19 .5	143	157	6	9	11	26	11	20	8	9
		(162)	(166)	(5)	(9)	(17)	(20)	(16)	(21)	(8)	(8)
	171	150	6	8	20	13	15	28	10	6	
78 .1	142	158	5	5	25	21	13	22	11	10	
	(157)	(154)	(6)	(7)	(23)	(17)	(14)	(25)	(11)	(8)	
	169	160	7	7	28	18	16	23	7	10	
313	183	166	3	8	18	26	22	30	6	7	
	(176)	(163)	(5)	(8)	(23)	(22)	(19)	(27)	(7)	(9)	
	155	178	6	15	18	15	14	17	6	8	
1250	152	144	9	7	13	25	23	25	6	8	
	(154)	(161)	(8)	(11)	(16)	(20)	(19)	(21)	(6)	(8)	
	146	201 *	6	9 *	17	22	21	25 *	8	7 *	
5000	143	192 *	11	6 *	14	24	13	25 *	6	5 *	
	(145)	(197 *)	(9)	(8 *)	(16)	(23)	(17)	(25 *)	(7)	(6 *)	
Judgement	—	—	—	—	—	—	—	—	—	—	
Specific Mutagenicity											
Positive Control	AF-2 (681)	2-AA (###)	NaN ₃ (263)	2-AA (209)	AF-2 (288)	2-AA (###)	AF-2 (411)	2-AA (488)	9-AA (739)	2-AA (163)	

Mutagenicity in Bacterial Test ; Negative

IARC Evaluation ; not yet cited

* Growth inhibition was observed.

Experimental Data-2

(B9603-2/3)

Conc. μ g/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2 $uvrA$		TA98		TA1537	
H ₂ O	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
	(157)	(165)	(10)	(10)	(20)	(27)	(13)	(24)	(6)	(8)
		179		15				31		7
		178		13				18		8
156	()	(179)	()	(14)	()	()	()	(25)	()	(8)
	163	186	14	9	20	22	21	22	10	8
	158	186	6	13	17	21	15	20	5	8
313	(161)	(186)	(10)	(11)	(19)	(22)	(18)	(21)	(8)	(8)
	152	178	6	9	23	31	20	31	8	5
	171	188	5	10	17	26	14	14	3	9
625	(162)	(183)	(6)	(10)	(20)	(29)	(17)	(23)	(6)	(7)
	183	176	10	8	15	22	18	28	6	7
	137	169	5	11	18	22	14	21	2	6
1250	(160)	(173)	(8)	(10)	(17)	(22)	(16)	(25)	(4)	(7)
	145	173	13	8	26	16	21	25	5	6
	172	164	6	6	28	29	18	30	3	9
2500	(159)	(169)	(10)	(7)	(27)	(23)	(20)	(28)	(4)	(8)
	160	188 *	7	9 *	17	33	14	24 *	5	10 *
	167	194 *	8	15 *	23	28	20	31 *	6	5 *
5000	(164)	(191 *)	(8)	(12 *)	(20)	(31)	(17)	(28 *)	(6)	(8 *)
Judgement	—	—	—	—	—	—	—	—	—	—
Specific Mutagenicity										
Positive Control	AF-2 (703)	2-AA (###)	NaN ₃ (215)	2-AA (188)	AF-2 (231)	2-AA (###)	AF-2 (410)	2-AA (414)	9-AA (766)	2-AA (159)

Experimental Data-3

Conc. μ g/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2 _{uvrA} /pKM101	
H ₂ O	S9-	S9+	S9-	S9+	S9-	S9+
	(312)	(367)	(324)	(330)	(53)	(82)
1 .22	330	364	305	379	56	86
	323	382	316	353	62	99
4 .88	(327)	(373)	(311)	(366)	(59)	(93)
	324	384	374	328	55	92
19 .5	335	361	326	340	75	94
	(330)	(373)	(350)	(334)	(65)	(93)
78 .1	312	350	316	361	57	93
	319	364	330	332	51	99
313	(316)	(357)	(323)	(347)	(54)	(96)
	340	388	337	373	60	109
1250	334	388	343	362	51	97
	(337)	(388)	(340)	(368)	(56)	(103)
5000	294	373	336	382	59	92
	314	305	364	390	57	82
Judgement	(304)	(339)	(350)	(386)	(58)	(87)
	297	350	378	334	60	112
Specific Mutagenicity	307	342	324	332	49	76
	(302)	(346)	(351)	(333)	(55)	(94)
Positive Control	307	362 *	344	373 *	59	98 *
	292	364 *	365	396 *	47	69 *
Positive Control	(300)	(363 *)	(355)	(385 *)	(53)	(84 *)
	BLM	2-AA	PA	2-AA	AF-2	2-AA
	(785)	(###)	(###)	(###)	(###)	(###)

Experimental Data-4 (B9603-3/3)

Conc. μ g/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2 _{uvrA} /pKM101	
H ₂ O	S9-	S9+	S9-	S9+	S9-	S9+
	(321)	(404)	(293)	(311)	(48)	(76)
156		412		314		54
	()	(390)	()	(306)	()	(61)
313	342	372	261	310	33	62
	348	405	279	334	48	89
625	(345)	(389)	(270)	(322)	(41)	(76)
	314	365	282	310	48	71
1250	341	414	310	340	46	67
	(328)	(390)	(296)	(325)	(47)	(69)
2500	309	358	292	389	63	77
	288	399	278	335	56	70
5000	(299)	(379)	(285)	(362)	(60)	(74)
	332	400	291	325	54	61
Judgement	300	372	286	320	52	79
	(316)	(386)	(289)	(323)	(53)	(70)
Specific Mutagenicity	293	404 *	309	382 *	43	83 *
	313	332 *	274	349 *	47	67 *
Positive Control	(303)	(368 *)	(292)	(366 *)	(45)	(75 *)
	BLM	2-AA	PA	2-AA	AF-2	2-AA
	(756)	(###)	(###)	(###)	(###)	(###)