

Chemical Name ; <u>1,3-Butadiene</u> Synonym ; <u>Buta-1,3-diene</u> <u>Butadiene</u> <u>Vinylethylene</u> <u>ブタジエン</u> Molecular Weight ; 54.09 Melting Point ; -109 °C[Aldrich] Boiling Point ; -4.5°C[Aldrich] Flashing Point ; -70 °C[CHCD] Molecular Formula ; C ₄ H ₆ Chemical Structure $\text{CH}_2=\text{CHCH}=\text{CH}_2$ CAS No. ; 106-99-0 MITI No. ; (2)-17 ML No. ; - Specified Chemical Substances ; - Source of Substance; Tokyo Kasei Kogyo Co., Ltd. Lot No. ; AO01(Experimental Data-1) AU01(Experimental Data-2) Purity ; >99% Vehicle ; Filtrated Air Exposure Condition ; 37°C, 48hr Culture Condition ; 37°C, 48hr	Conc. %	Number of Revertants/plate									
		Base-substitution						Frame-shift			
		TA100		TA1535		WP2uvrA		TA98		TA1537	
		S9-	S9+/40%	S9-	S9+/40%	S9-	S9+/40%	S9-	S9+/40%	S9-	S9+/40%
	Air	(136)	(124)	(23)	(11)	(49)	(30)	(11)	(29)	(8)	(18)
		81	105	11	28	24	31	10	29	4	10
		98	151	12	31	35	32	12	30	5	8
	3	(90)	(128)	(12)	(30)	(30)	(32)	(11)	(30)	(5)	(9)
		108	134	17	39	40	38	10	21	7	13
		108	151	11	36	32	31	11	25	5	14
	7	(108)	(143)	(14)	(38)	(36)	(35)	(11)	(23)	(6)	(14)
		86		14		35		9		7	
		85		14		29		12		7	
11	(86)		(14)		(32)		(11)		(7)		
		120		67		44		25		11	
		128		62		30		30		15	
12		(124)		(65)		(37)		(28)		(13)	
	77		9		33		8		5		
	76		16		56		17		6		
22	(77)		(13)		(45)		(13)		(6)		
		159		96		33		24		14	
		124		97		43		33		12	
23		(142)		(97)		(38)		(29)		(13)	
	88		19		37		13		5		
	81		15		33		7		4		
53	(85)		(17)		(35)		(10)		(5)		
		234		182		34		26		12	
		228		134		50		24		8	
58		(231)		(158)		(42)		(25)		(10)	
Judgement	-	+	-	+	-	-	-	-	-	-	
Specific Mutagenicity #		58%		3%							
Positive Control	AF-2 (418)	2-AA (418)	NaN ₃ (324)	2-AA (338)	AF-2 (273)	2-AA (391)	AF-2 (363)	2-AA (101)	9-AA (665)	2-AA (76)	

The concentration which was two times of the negative controle value was shown.

Experimental Data-2

(B8601-2/2)

Conc. %	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2 _{uvrA}		TA98		TA1537	
Air	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
	(159)	(162)	(13)	(12)	(15)	(22)	(15)	(28)	(12)	(18)
1 .5	207	143	23	19	23	42	25	37	10	32
	162	179	22	17	23	20	26	36	17	34
3 .8	(185)	(161)	(23)	(18)	(23)	(31)	(26)	(37)	(14)	(33)
		173		27		29		44		36
4 .0		179		28		31		41		37
		(176)		(28)		(30)		(43)		(37)
6 .8	177		13		26		23		11	
	189		30		13		19		11	
6 .9	(183)		(22)		(20)		(21)		(11)	
	168		20		16		17		15	
16	153		23		21		12		14	
	(161)		(22)		(19)		(15)		(14)	
18		186		31		22		27		26
		150		27		26		45		36
39		(168)		(29)		(24)		(36)		(31)
	121		27		15		17		11	
40	186		17		17		22		8	
	(154)		(22)		(16)		(20)		(10)	
40		164		27		39		45		31
		159		27		39		34		34
40		(162)		(27)		(39)		(40)		(33)
		148		33		16		40		29
40		149		41		30		41		25
		(149)		(37)		(23)		(41)		(27)
40	144		28		15		13		8	
	156		28		13		19		8	
40	(150)		(28)		(14)		(16)		(8)	
	Judgement	-	-	-	+	-	-	-	-	-
Specific Mutagenicity #				3.8%						
Positive Control	AF-2 (735)	2-AA (810)	NaN ₃ (178)	2-AA (229)	AF-2 (256)	2-AA/20 (1299)	AF-2 (539)	2-AA (261)	9-AA (194)	2-AA (708)