1,4-Dibromobutane (1,4-ジブロモブタン)

Chemical Name: 1,4-Dibromobutane
Synonym: Tetramethylene dibromide
Butane, 1,4-dibromo-
Molecular weight: 215.92
Melting point: -20℃
Boiling point: 197~198℃, 110℃ (58 mHg)
76℃ (11 mmHg)
Chemical Structure

$$Br-CH_2-CH_2-CH_2-CH_2-Br$$

CAS No : 110-52-1
MITI No: (2)-59, (9)-2008
Source of Substance:Tokyo Kasei Kogyo Co.Ltd
Lot.No. : FDZ01
Purity : 98 %
Vehicle : DMSO

Mutagenicity
in Bacterial Test : Positive

IARC Evaluation : not yet cited

Experimental Data

Con. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA		TA98		TA1537	
	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
DMSO	(191)	(166)	(27)	(41)	(28)	(37)	(15)	(22)	(9)	(10)
	152	162	37	40	40	37	16	23	6	13
	180	145	18	32	29	36	15	23	7	9
0.0763	(166)	(154)	(28)	(36)	(35)	(37)	(16)	(23)	(7)	(11)
	173	151	29	26	37	31	20	33	10	7
	152	157	32	33	23	32	17	16	6	5
0.305	(163)	(154)	(31)	(30)	(30)	(32)	(19)	(25)	(8)	(6)
	133	157	20	53	29	29	15	30	13	10
	146	150	37	39	25	34	11	31	9	7
1.22	(140)	(154)	(29)	(46)	(27)	(32)	(13)	(31)	(11)	(9)
	143	180	32	36	17	39	15	22	8	9
	153	148	31	28	45	48	22	28	7	7
4.88	(148)	(164)	(32)	(32)	(31)	(44)	(19)	(25)	(8)	(8)
	142	177	41	52	32	34	33	24	13	8
	156	173	41	44	37	33	14	34	14	6
19.5	(149)	(175)	(41)	(48)	(35)	(34)	(24)	(29)	(14)	(7)
	236	218	97*	74	48	55	20	21	7	9
	206	179	68*	71	40	44	22	24	8	9
78.1	(221)	(199)	(83*)	(73)	(44)	(50)	(21)	(23)	(8)	(9)
	252*	293	45*	123*	76	108	17*	18*	8*	8*
	214*	352	81*	130*	77	88	9*	21*	5*	11*
313	(233*)	(323)	(63*)	(127*)	(77)	(98)	(13*)	(20*)	(7*)	(10*)
	0*	0*	0*	0*	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*	0*	0*	0*	0*
1250	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
5000	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
Judgement	−	−	+	+	+	+	−	−	−	−
Specific Mutagenicity			717	275	157	195				
Positive Control	AF2 (860)	2AA (1141)	NaN_3 (300)	2AA (289)	AF2 (255)	2AA (886)	AF2 (526)	2AA (354)	9AA (438)	2AA (187)

Experimental Data

Con. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA		TA98		TA1537	
	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
DMSO	(170)	(151)	(15)	(13)	(19)	(24)	(25)	(29)	(12)	(15)
			21							
			31							
2.44			(26)							
	170		25	26			29	39	16	17
	177		28	21			24	36	14	26
4.88	(174)		(27)	(24)			(27)	(38)	(15)	(22)
	158	153	21	20	24	28	21	29	17	26
	173	185	28	27	31	38	30	30	18	21
9.77	(166)	(169)	(25)	(24)	(28)	(33)	(26)	(30)	(18)	(24)
	174	133	24	37	16	29	29	32	16	16
	185	152	27	29	32	21	28	31	17	17
19.5	(180)	(143)	(26)	(33)	(24)	(25)	(29)	(32)	(17)	(17)
	171	177	32	45	36	44	20	43	15	29
	169	195	48	48	37	38	13	33	16	16
39.1	(170)	(186)	(40)	(47)	(37)	(41)	(17)	(38)	(16)	(23)
	181	187	51	54	32	45	22	31	15	31
	208	201	59	77	40	48	15	32	22	23
78.1	(195)	(194)	(55)	(66)	(36)	(47)	(19)	(32)	(19)	(27)
	256	254	87*	105	54	61	23	31	20	30
	256	258	126*	113	61	66	26	32	20	18
156	(256)	(256)	(107*)	(109)	(58)	(64)	(25)	(32)	(20)	(24)
	243*	311	56*	129	91	112	33*	38	17*	21
	255*	312	56*	167	82	112	26*	43	15*	26
313	(249*)	(312)	(56*)	(148)	(87)	(112)	(30*)	(41)	(16*)	(24)
	0*	0*		0*	0*	33*	0*	0*	0*	0*
	0*	0*		0*	0*	23*	0*	0*	0*	0*
625	(0*)	(0*)		(0*)	(0*)	(28*)	(0*)	(0*)	(0*)	(0*)
1250		(0*)			(0*)	(0*)				
Judgement	−	+	+	+	+	+	−	−	−	−
Specific Mutagenicity		514	639	1030	250	281				
Positive Control	AF2	2AA	NaN_3	2AA	AF2	2AA	AF2	2AA	9AA	2AA
	(905)	(1437)	(491)	(325)	(292)	(850)	(545)	(366)	(413)	(279)

Experimental Data				
Con. μg/plate	Number of Revertants/plate			
	Base-substitution			
	TA100		TA1535	
	S9-	S9+	S9-	S9+
DMSO	(141)	(106)	(10)	(13)
			14	
			13	
2.44	( )	( )	(14)	( )
	146		20	13
	184		17	22
4.88	(165)	( )	(19)	(18)
	145	108	24	10
	156	96	28	16
9.77	(151)	(102)	(26)	(13)
	129	155	23	26
	130	124	32	22
19.5	(130)	(140)	(28)	(24)
	172	134	43	61
	136	123	53	29
39.1	(154)	(129)	(48)	(45)
	178	193	68	76
	222	198	68	57
78.1	(200)	(196)	(68)	(67)
	267	240	143	130
	241	214	112	117
156	(254)	(227)	(128)	(124)
	223*	233	28*	93
	219*	215	31*	78
313	(221*)	(224)	(30*)	(86)
625	(0*)	(0*)	( )	(0*)
1250	( )	(0*)	( )	( )
Judgement	−	+	+	+
Specific Mutagenicity		776	1640	818
Positive Control	AF2	2AA	NaN_3	2AA
	(1013)	(1286)	(158)	(234)