

Bis(2-chloroethyl) ether

[ビス(2-クロロエチル)エーテル]

Experimental Data - 1

(B9402-1/5)

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Chemical Name; Bis(2-chloroethyl) ether
 Synonym ; 2,2'-Dichloroethyl ether
 1,1'-Oxybis(2-chloroethane)
 Di-2-chloroethyl ether
 2,2'-ジクロロジエチルエーテル
 1,1'-オキシビス(2-クロロエタン)
 ジ-2-クロロエチルエーテル

Molecular Weight ; 143.01
 Melting Point ; - 47 °C [Aldrich]
 - 50 °C [Merck]
 Boiling Point ; 177-178 °C, 66 °C (12mmHg) [CHCD]
 65 - 67 °C (15mmHg) [Aldrich]
 Flashing Point ; 55 °C [CHCD, Aldrich, Merck]
 63 °C (c. c) [Merck]
 Molecular Formula; C₄H₈Cl₂O

Chemical Structure

ClCH₂CH₂OCH₂CH₂Cl

CAS No. ; 111-44-4
 MITI No. ; (2)-382
 ML No. ; -
 Specified Chemical Substances; -

Source of Substance; Tokyo Kasei Kogyo Co., Ltd.
 Lot No. ; FGC01
 Purity ; 99 %

Vehicle ; Dehydrated DMSO

Mutagenicity in Bacterial Test ; **Positive**

IARC Evaluation ; not yet cited

Conc. µg/plate	Number of Revertants/plate								
	Base-substitution								
	TA100			TA1535			WP2uvrA		
	S9-	RatS9+	HamsterS9+	S9-	RatS9+	HamsterS9+	S9-	RatS9+	HamsterS9+
DMSO	(122)	(135)	(150)	(16)	(20)	(27)	(20)	(27)	(19)
	137			25			9		
	90			10			18		
19.5	(114)			(18)			(14)		
	113	133	145	22	29	20	18	22	16
	126	158	153	24	21	22	14	23	15
39.1	(120)	(146)	(149)	(23)	(25)	(21)	(16)	(23)	(16)
	112	133	167	25	18	23	20	29	26
	121	133	165	15	23	18	18	17	14
78.1	(117)	(133)	(166)	(20)	(21)	(21)	(19)	(23)	(20)
	126	150	179	15	15	23	16	23	28
	121	137	155	18	25	24	25	24	20
156	(124)	(144)	(167)	(17)	(20)	(24)	(21)	(24)	(24)
	130	151	158	20	23	23	13	26	28
	142	171	169	18	25	21	18	14	20
313	(136)	(161)	(164)	(19)	(24)	(22)	(16)	(20)	(24)
	117	160	153	24	31	29	21	22	23
	137	176	152	20	30	32	20	11	23
625	(127)	(168)	(153)	(22)	(31)	(31)	(21)	(17)	(23)
	137	156	142	18	30	37	18	32	20
	127	162	163	30	38	43	21	25	25
1250	(132)	(159)	(153)	(24)	(34)	(40)	(20)	(29)	(23)
	166	202	191	41	41	52	17	38	36
	169	185	191	38	32	44	22	36	33
2500	(168)	(194)	(191)	(40)	(37)	(48)	(20)	(37)	(35)
	71*	99*	152*	15*	24*	40*	28*	29	46
	44*	134*	192	20*	46*	47*	28*	29	31
5000	(58*)	(117*)	(172*)	(18*)	(35*)	(44*)	(28*)	(29)	(39)
		0*	0*		0*	0*		14*	30*
		0*	0*		0*	0*		17*	36*
10000		(0*)	(0*)		(0*)	(0*)		(16*)	(33*)
Judgement	-	-	-	+	-	-	-	-	+
Specific Mutagenicity				9.60					4.00
Positive Control	AF-2 (889)	2-AA (1208)	2-AA (3212)	NaN ₃ (442)	2-AA (342)	2-AA (518)	AF-2 (341)	2-AA (1082)	2-AA (1454)

Experimental Data - 1

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Conc. µg/plate	Number of Revertants/plate					
	Frame-shift					
	TA98			TA1537		
	S9-	RatS9+	HamsterS9+	S9-	RatS9+	HamsterS9+
	(18)	(21)	(23)	(4)	(11)	(9)
DMSO	21			2		
	13			7		
19.5	(17)			(5)		
	13	28	24	1	8	2
	9	20	26	7	6	2
39.1	(11)	(24)	(25)	(4)	(7)	(2)
	13	23	22	7	8	2
	13	21	24	3	7	6
78.1	(13)	(22)	(23)	(5)	(8)	(4)
	14	14	29	3	8	8
	8	18	28	3	9	5
156	(11)	(16)	(29)	(3)	(9)	(7)
	10	26	22	3	3	3
	9	29	26	2	5	6
313	(10)	(28)	(24)	(3)	(4)	(5)
	10	13	29	6	7	2
	9	25	30	5	14	7
625	(10)	(19)	(30)	(6)	(11)	(5)
	15	22	16	7	3	5
	20	30	31	8	9	5
1250	(18)	(26)	(24)	(8)	(6)	(5)
	16	22	37	10	8	5
	21	34	28	8	6	5
2500	(19)	(28)	(33)	(9)	(7)	(5)
	2*	20*	38	6*	8	8*
	6*	20*	16	7*	7	9*
5000	(4*)	(20*)	(27)	(7*)	(8)	(9*)
		0*	0*		0*	0*
		0*	0*		0*	0*
10000		(0*)	(0*)		(0*)	(0*)
Judgement	—	—	—	—	—	—
Specific Mutagenicity						
Positive Control	AF-2 (356)	2-AA (273)	2-AA (847)	9-AA (788)	2-AA (251)	2-AA (873)

(same experiment with next page)

Conc. µg/plate	Number of Revertants/plate								
	Base-substitution								
	TA100			TA1535			WP2uvrA		
	S9-	RatS9+	HamsterS9+	S9-	RatS9+	HamsterS9+	S9-	RatS9+	HamsterS9+
	(107)	(124)	(120)	(9)	(10)	(14)	(27)	(38)	(33)
DMSO	106			7			32		
	122			16			18		
313	(114)			(12)			(25)		
	112	138	137	8	14	18	17		
	127	128	136	7	11	22	24		
625	(120)	(133)	(137)	(8)	(13)	(20)	(21)		
	100	145	149	13	21	24	25	41	43
	111	144	139	18	20	16	24	49	44
1250	(106)	(145)	(144)	(16)	(21)	(20)	(24)	(45)	(44)
	146	163	148	20	17	24	20	29	40
	159	141	178	20	28	25	29	47	46
1875	(153)	(152)	(163)	(20)	(23)	(25)	(25)	(38)	(43)
	155	157	180	23	29	39	41	44	36
	155	169	202	28	31	34	30	29	43
2500	(155)	(163)	(191)	(26)	(30)	(37)	(36)	(37)	(40)
	79*	180	173	20*	37	41	41	49	39
	97*	185	170	14*	22	36	31	51	54
3750	(88*)	(183)	(172)	(17*)	(30)	(39)	(36)	(50)	(47)
	78*	119*	120*	16*	18*	21*	24*	32*	55
	61*	108*	133*	0*	17*	26*	21*	40*	36
5000	(70*)	(114*)	(127*)	(8*)	(18*)	(24*)	(23*)	(36*)	(46)
		0*	0*		0*	0*		13*	13*
		0*	0*		0*	0*		11*	3*
7500		(0*)	(0*)		(0*)	(0*)		(12*)	(8*)
								0*	0*
								0*	0*
10000								(0*)	(0*)
Judgement	-	-	-	+	+	+	-	-	-
Specific Mutagenicity				6.80	8.80	9.20			
Positive Control	AF-2 (856)	2-AA (1196)	2-AA (3545)	NaN ₃ (366)	2-AA (297)	2-AA (582)	AF-2 (351)	2-AA (1111)	2-AA (1447)

Experimental Data - 2

(B9402-4/5)

(same experiment with previous page)

Conc. µg/plate	Number of Revertants/plate					
	Frame-shift					
	TA98			TA1537		
	S9-	RatS9+	HamsterS9+	S9-	RatS9+	HamsterS9+
	(16)	(26)	(24)	(14)	(19)	(18)
DMSO	16			15		
	23			14		
313	(20)			(15)		
	17	26		20		14
	15	14		14		17
625	(16)	(18)		(17)		(16)
	15	21	30	7	16	17
	17	20	26	21	22	22
1250	(16)	(21)	(28)	(14)	(19)	(20)
	13	20	21	18	16	20
	16	24	23	17	24	21
1875	(15)	(22)	(22)	(18)	(20)	(21)
	11	29	20	11	20	22
	18	25	28	18	28	22
2500	(15)	(27)	(24)	(15)	(24)	(22)
	13*	29	31	22	20	25
	17*	26	17	14	20	24
3750	(15*)	(28)	(24)	(18)	(20)	(25)
	1*	21*	18*	2*	7*	14*
	6*	11*	20*	3*	8*	8*
5000	(4*)	(16*)	(19*)	(3*)	(8*)	(11*)
		0*	0*		0*	0*
		0*	0*		0*	0*
7500		(0*)	(0*)		(0*)	(0*)
			0*		0*	
			0*		0*	
10000			(0*)		(0*)	
Judgement	—	—	—	—	—	—
Specific Mutagenicity						
Positive	AF-2	2-AA	2-AA	9-AA	2-AA	2-AA
Control	(345)	(286)	(1050)	(731)	(217)	(848)

Conc. µg/plate	Number of Revertants/plate								
	Base-substitution						Frame-shift		
	TA1535			WP2uvrA			TA1537		
	S9-	RatS9+	HamsterS9+	S9-	RatS9+	HamsterS9+	S9-	RatS9+	HamsterS9+
	(13)	(20)	(14)	(23)	(32)	(23)	(8)	(8)	(8)
DMSO	13	21	17	33	32	33	14	14	7
	16	23	25	22	32	29	7	11	6
313	(15)	(22)	(21)	(28)	(32)	(31)	(11)	(13)	(7)
	23	20	23	25	37	26	6	22	9
	22	11	22	20	33	41	6	8	7
625	(23)	(16)	(23)	(23)	(35)	(34)	(6)	(15)	(8)
	24	20	25	40	40	36	7	13	8
	20	24	26	33	39	33	18	15	10
1250	(22)	(22)	(26)	(37)	(40)	(35)	(13)	(14)	(9)
	24	17	31	23	37	48	5	5	14
	20	25	39	30	38	49	10	8	7
1875	(22)	(21)	(35)	(27)	(38)	(49)	(8)	(7)	(11)
	29	34	28	15	40	45	9	14	7
	31	48	32	26	33	54	9	14	10
2500	(30)	(41)	(30)	(21)	(37)	(50)	(9)	(14)	(9)
	33*	32	39	26	32	43	8	13	7
	37*	48	34	39	48	38	10	13	8
3750	(35*)	(40)	(37)	(33)	(40)	(41)	(9)	(13)	(8)
	0*	0*	0*	26*	31*	39*	0*	0*	0*
	0*	0*	0*	32*	23*	20*	0*	0*	0*
5000	(0*)	(0*)	(0*)	(29*)	(27*)	(30*)	(0*)	(0*)	(0*)
Judgement	+	+	+	-	-	+	-	-	-
Specific Mutagenicity	6.80	8.40	11.2			13.9			
Positive Control	NaN ₃ (383)	2-AA (296)	2-AA (464)	AF-2 (256)	2-AA (1205)	2-AA (1474)	9-AA (837)	2-AA (203)	2-AA (875)