

2,2-Dimethyl-1,3-propanediol
 (2,2-ジメチル-1,3-プロパンジオール)

Experimental Data-1

(B9611-1/3)

Chemical Name	; <u>2,2-Dimethyl-1,3-propanediol</u>	
Synonym	; <u>2,2-Dimethylpropane-1,3-diol</u> <u>Neopentyl glycol</u> ネオペンチルグリコール	
Molecular Weight	; 104.15	
Melting Point	; 129°C [CHCD]	
Boiling Point	; 206°C(747mmHg)[CHCD]	
Flashing Point	; 107°C [Aldrich]	
Molecular Formula	; C ₅ H ₁₂ O ₂	
Chemical Structure	(CH ₃) ₂ C(CH ₂ OH) ₂	
CAS No.	; 126-30-7	
MITI No.	; (2)-240	
ML No.	; -	
Specified Chemical Substances	; -	
Source of Substance	; Tokyo Kasei Kogyo Co., Ltd.	
Lot No.	; GE01	
Purity	; 99.5%	
Vehicle	; H ₂ O	

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+
	(150)	(142)	(7)	(10)	(18)	(23)	(14)	(22)	(6)	(11)
1 .22	150	142	6	6	17	15	8	18	3	6
	150	164	8	8	15	24	14	21	3	13
4 .88	(150)	(153)	(7)	(7)	(16)	(20)	(11)	(20)	(3)	(10)
	142	138	7	7	17	18	8	28	6	8
19 .5	144	151	14	9	17	24	16	25	7	6
	(143)	(145)	(11)	(8)	(17)	(21)	(12)	(27)	(7)	(7)
78 .1	158	141	7	9	18	26	15	18	3	6
	162	141	3	11	8	20	14	21	7	11
313	(160)	(141)	(5)	(10)	(13)	(23)	(15)	(20)	(5)	(9)
	148	137	7	11	13	17	16	18	9	9
1250	172	143	5	10	15	22	16	32	2	11
	(160)	(140)	(6)	(11)	(14)	(20)	(16)	(25)	(6)	(10)
5000	142	143	10	9	16	28	14	11	5	11
	156	156	8	3	24	18	10	15	5	11
Judgement	(149)	(150)	(9)	(6)	(20)	(23)	(12)	(13)	(5)	(11)
	174	163	10	9	17	22	9	29	5	13
Specific Mutagenicity	166	157	5	6	17	26	16	25	2	13
	(170)	(160)	(8)	(8)	(17)	(24)	(13)	(27)	(4)	(13)
Positive Control	160	157	8	9	22	30	15	33	5	16
	176	166	9	8	23	29	16	16	7	14
AF-2	(168)	(162)	(9)	(9)	(23)	(30)	(16)	(25)	(6)	(15)
	-	-	-	-	-	-	-	-	-	-
2-AA	-	-	-	-	-	-	-	-	-	-
	-	-	-	-	-	-	-	-	-	-
NaN ₃	-	-	-	-	-	-	-	-	-	-
	-	-	-	-	-	-	-	-	-	-
9-AA	-	-	-	-	-	-	-	-	-	-
	-	-	-	-	-	-	-	-	-	-
2-AA	-	-	-	-	-	-	-	-	-	-
	-	-	-	-	-	-	-	-	-	-

Mutagenicity in Bacterial Test ; Negative

IARC Evaluation ; not yet cited

Experimental Data-2

(B9611-2/3)

Conc. μ g/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA		TA98		TA1537	
H ₂ O	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
	(136)	(150)	(8)	(9)	(25)	(23)	(13)	(20)	(6)	(11)
	148	153	13	11	18	36	10	21	5	14
313	117	156	5	11	18	21	11	24	6	9
	(133)	(155)	(9)	(11)	(18)	(29)	(11)	(23)	(6)	(12)
	148	151	7	9	15	22	6	26	6	11
625	116	143	6	10	17	22	11	24	6	10
	(132)	(147)	(7)	(10)	(16)	(22)	(9)	(25)	(6)	(11)
	157	122	8	7	22	24	11	23	8	6
1250	126	141	8	11	15	26	11	21	9	5
	(142)	(132)	(8)	(9)	(19)	(25)	(11)	(22)	(9)	(6)
	151	136	8	9	15	20	11	28	5	10
2500	138	130	8	11	22	18	11	25	8	10
	(145)	(133)	(8)	(10)	(19)	(19)	(11)	(27)	(7)	(10)
	149	153	11	10	14	18	10	17	9	15
5000	153	138	10	8	18	17	22	26	10	9
	(151)	(146)	(11)	(9)	(16)	(18)	(16)	(22)	(10)	(12)
Judgement	—	—	—	—	—	—	—	—	—	—
Specific Mutagenicity										
Positive Control	AF-2 (625)	2-AA (1163)	NaN ₃ (265)	2-AA (223)	AF-2 (212)	2-AA (1062)	AF-2 (484)	2-AA (449)	9-AA (709)	2-AA (162)

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+
	(245)	(347)	(320)	(325)	(44)	(72)
1 .22	292	306	366	346	56	70
	278	328	293	311	59	77
	(285)	(317)	(330)	(329)	(58)	(74)
4 .88	287	353	352	328	53	66
	262	354	349	278	62	76
	(275)	(354)	(351)	(303)	(58)	(71)
19 .5	282	362	365	337	59	85
	274	336	366	338	61	64
	(278)	(349)	(366)	(338)	(60)	(75)
78 .1	269	406	354	295	52	90
	273	371	336	342	51	81
	(271)	(389)	(345)	(319)	(52)	(86)
313	282	346	347	323	61	56
	261	349	396	319	63	82
	(272)	(348)	(372)	(321)	(62)	(69)
1250	274	387	331	329	60	79
	273	356	377	314	45	76
	(274)	(372)	(354)	(322)	(53)	(78)
5000	280	368	359	332	59	92
	271	332	316	335	47	93
	(276)	(350)	(338)	(334)	(53)	(93)
Judgement	—	—	—	—	—	—
Specific Mutagenicity						
Positive Control	BLM (735)	2-AA (1343)	PA (1812)	2-AA (1415)	AF-2 (1407)	2-AA (1011)

Experimental Data-4

(B9611-3/3)

Conc. μ g/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2 ^{uvrA} /pKM101	
H ₂ O	S9-	S9+	S9-	S9+	S9-	S9+
	(296)	(393)	(291)	(306)	(44)	(65)
313	312	407	343	350	39	83
	293	384	343	336	40	74
	(303)	(396)	(343)	(343)	(40)	(79)
625	276	367	311	389	48	77
	286	382	335	348	59	75
	(281)	(375)	(323)	(369)	(54)	(76)
1250	299	414	341	336	55	94
	298	344	323	324	38	74
	(299)	(379)	(332)	(330)	(47)	(84)
2500	286	377	305	348	54	83
	306	383	331	332	49	97
	(296)	(380)	(318)	(340)	(52)	(90)
5000	282	380	367	358	26	78
	255	354	368	309	43	71
	(269)	(367)	(368)	(334)	(35)	(75)
Judgement	—	—	—	—	—	—
Specific Mutagenicity						
Positive Control	BLM (734)	2-AA (1051)	PA (1694)	2-AA (1307)	AF-2 (791)	2-AA (885)