

Experimental Data-1

(B9914-1/2)

2-Methylpentane-2,4-diol (2-メチルペンタン-2,4-ジオール)

Chemical Name	: 2-Methylpentane-2,4-diol
Synonym	: Hexylene glycol
Molecular Weight	: 118.18
Melting Point	: -40°C [Aldrich]
Boiling Point	: 198°C [Merck]
Flashing Point	: 93°C(o.c.)[Merck]
Molecular Formula	: C <sub>6</sub> H <sub>14</sub> O <sub>2</sub>
Chemical Structure:	$  \begin{array}{c}  \text{CH}_3 \\    \\  \text{H}_3\text{C}-\text{C}-\text{CH}_2-\text{CH}-\text{CH}_3 \\    \quad \quad   \\  \text{OH} \quad \quad \text{OH}  \end{array}  $
CAS No.	: 107-41-5
METI No.	: (2)-240
MHLW No.	: -
Specified Chemical Substances	: -
Source of Substance	: Tokyo Kasei Kogyo Co., Ltd.
Lot No.	: GG01-AK
Purity	: >99%
Vehicle	: Distilled H <sub>2</sub> O

Mutagenicity in Bacterial Test: Negative

IARC Evaluation : not yet cited

Conc. μ g/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA/pKM101		TA98		TA1537	
H <sub>2</sub> O	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
		( 108 )	( 132 )	( 11 )	( 6 )	( 71 )	( 101 )	( 19 )	( 26 )	( 5 )
1 .22	114	121	7	3	56	92	33	34	5	14
	111	115	6	7	63	81	30	17	3	18
	( 113 )	( 118 )	( 7 )	( 5 )	( 60 )	( 87 )	( 32 )	( 26 )	( 4 )	( 16 )
4 .88	124	134	6	17	79	112	21	33	8	5
	111	114	6	3	92	116	15	25	7	9
	( 118 )	( 124 )	( 6 )	( 10 )	( 86 )	( 114 )	( 18 )	( 29 )	( 8 )	( 7 )
19 .5	105	120	11	5	32	101	29	36	7	8
	101	129	10	13	113	102	22	33	6	6
	( 103 )	( 125 )	( 11 )	( 9 )	( 73 )	( 102 )	( 26 )	( 35 )	( 7 )	( 7 )
78 .1	117	124	7	9	83	109	13	36	10	7
	114	126	15	5	81	104	16	26	2	13
	( 116 )	( 125 )	( 11 )	( 7 )	( 82 )	( 107 )	( 15 )	( 31 )	( 6 )	( 10 )
313	92	141	9	7	91	100	26	26	7	14
	102	149	7	6	89	97	15	25	5	15
	( 97 )	( 145 )	( 8 )	( 7 )	( 90 )	( 99 )	( 21 )	( 26 )	( 6 )	( 15 )
1250	117	121	13	6	75	90	17	16	8	9
	105	113	8	10	92	94	20	22	3	6
	( 111 )	( 117 )	( 11 )	( 8 )	( 84 )	( 92 )	( 19 )	( 19 )	( 6 )	( 8 )
5000	104	141	11	10	75	104	18	13	6	9
	85	121	6	8	93	98	14	23	8	7
	( 95 )	( 131 )	( 9 )	( 9 )	( 84 )	( 101 )	( 16 )	( 18 )	( 7 )	( 8 )
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive Control	AF-2 ( 605 )	2-AA ( 1081 )	NaN <sub>3</sub> ( 356 )	2-AA ( 241 )	AF-2 ( 1376 )	2-AA ( 733 )	AF-2 ( 444 )	2-AA ( 466 )	9-AA ( 354 )	2-AA ( 234 )

Experimental Data-2

(B9914-2/2)

Conc. μ g/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2 <i>uvrA</i> /pKM101		TA98		TA1537	
	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
H <sub>2</sub> O	( 118 )	( 117 )	( 10 )	( 8 )	( 75 )	( 102 )	( 15 )	( 22 )	( 7 )	( 14 )
313	109	145	9	9	85	90	20	32	6	10
	112	119	8	13	61	87	18	31	8	8
	( 111 )	( 132 )	( 9 )	( 11 )	( 73 )	( 89 )	( 19 )	( 32 )	( 7 )	( 9 )
625	134	126	8	7	68	94	11	32	5	7
	115	126	13	6	66	108	17	24	7	15
	( 125 )	( 126 )	( 11 )	( 7 )	( 67 )	( 101 )	( 14 )	( 28 )	( 6 )	( 11 )
1250	105	119	3	6	62	91	14	17	8	14
	144	142	17	5	76	101	14	21	5	11
	( 125 )	( 131 )	( 10 )	( 6 )	( 69 )	( 96 )	( 14 )	( 19 )	( 7 )	( 13 )
2500	114	116	10	7	79	92	10	17	8	14
	120	117	8	6	60	106	14	23	7	11
	( 117 )	( 117 )	( 9 )	( 7 )	( 70 )	( 99 )	( 12 )	( 20 )	( 8 )	( 13 )
5000	119	121	14	5	83	85	14	23	5	8
	117	104	9	11	56	82	16	26	10	13
	( 118 )	( 113 )	( 12 )	( 8 )	( 70 )	( 84 )	( 15 )	( 25 )	( 8 )	( 11 )
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive Control	AF-2 ( 732 )	2-AA ( 1352 )	NaN <sub>3</sub> ( 469 )	2-AA ( 262 )	AF-2 ( 1040 )	2-AA ( 796 )	AF-2 ( 466 )	2-AA ( 464 )	9-AA ( 434 )	2-AA ( 221 )