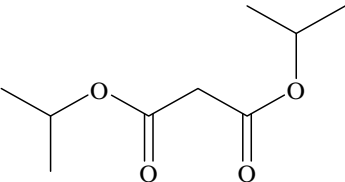


Chemical Name	: <u>Diisopropyl malonate</u>
Synonym	: <u>Malonic acid, diisopropyl ester</u> <u>Propanedioic acid, diisopropyl ester</u> ジイソプロピルマロナート
Molecular Weight	: 188.22
Melting Point	: -
Boiling Point	: 93-95°C [Aldrich]
Flashing Point	: 89°C [Aldrich]
Molecular Formula	: C <sub>9</sub> H <sub>16</sub> O <sub>4</sub>
Chemical Structure	
CAS No.	: 13195-64-7
MITI No.	: (2)-2549
ML No.	: -
Specified Chemical Substances	: -
Source of Substance	: Tokyo Kasei Kogyo Co., Ltd.
Lot No.	: AL-01
Purity	: >99%
Vehicle	: DMSO

Conc. μ g/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA/pKM101		TA98		TA1537	
DMSO	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
	( 164 )	( 154 )	( 9 )	( 8 )	( 40 )	( 57 )	( 13 )	( 20 )	( 6 )	( 8 )
	170	197	8	10	22	45	14	24	11	9
1 .22	( 176 )	( 192 )	( 11 )	( 10 )	( 34 )	( 52 )	( 14 )	( 23 )	( 10 )	( 8 )
	181	197	5	5	40	66	16	20	6	10
4 .88	( 177 )	( 181 )	( 6 )	( 9 )	( 36 )	( 61 )	( 19 )	( 22 )	( 6 )	( 7 )
	174	187	10	10	37	84	15	17	6	15
19 .5	( 175 )	( 192 )	( 9 )	( 10 )	( 41 )	( 80 )	( 14 )	( 24 )	( 8 )	( 12 )
	184	159	6	9	57	76	10	21	5	8
78 .1	( 168 )	( 157 )	( 7 )	( 10 )	( 47 )	( 73 )	( 12 )	( 23 )	( 4 )	( 9 )
	166	162	9	11	34	86	9	28	6	10
313	( 170 )	( 182 )	( 8 )	( 11 )	( 38 )	( 71 )	( 13 )	( 25 )	( 6 )	( 9 )
	173	201	7	10	41	56	17	21	5	7
1250	( 155 )	( 167 )	( 7 *)	( 11 )	( 41 )	( 70 )	( 13 )	( 21 )	( 7 )	( 6 )
	166	166	2 *	10	41	69	13	22	9	7
5000	( 0 *)	( 89 *)	( 0 *)	( 11 *)	( 0 *)	( 36 *)	( 0 *)	( 16 *)	( 0 *)	( 7 *)
	0 *	92	0 *	8	0 *	39	0 *	22	0 *	6
	0 *	86	0 *	13	0 *	33	0 *	10	0 *	7
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive Control	AF-2 ( 658 )	2-AA ( 1143 )	NaN <sub>3</sub> ( 324 )	2-AA ( 243 )	AF-2 ( 663 )	2-AA ( 708 )	AF-2 ( 390 )	2-AA ( 383 )	9-AA ( 558 )	2-AA ( 152 )

Mutagenicity in Bacterial Test ; Negative

\* Growth inhibition was observed.

IARC Evaluation ; not yet cited

Experimental Data-2

(B9824-2/2)

Conc. $\mu$ g/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA/pKM101		TA98		TA1537	
DMSO	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
	( 160 )	( 169 )	( 12 )	( 13 )	( 45 )	( 59 )	( 13 )	( 22 )	( 6 )	( 6 )
19 .5			14 9 ( 12 )							
39 .1			14 11 ( 13 )							
78 .1	151	176	8	14	31	55	16	15	5	5
	163 ( 157 )	167 ( 172 )	13 ( 11 )	15 ( 15 )	26 ( 29 )	67 ( 61 )	14 ( 15 )	25 ( 20 )	5 ( 5 )	10 ( 8 )
156	173	178	9	15	46	66	21	28	6	6
	178 ( 176 )	186 ( 182 )	13 ( 11 )	9 ( 12 )	47 ( 47 )	75 ( 71 )	15 ( 18 )	23 ( 26 )	3 ( 5 )	6 ( 6 )
313	179	150	11	14	52	55	10	22	7	8
	152 ( 166 )	186 ( 168 )	10 ( 11 )	13 ( 14 )	41 ( 47 )	67 ( 61 )	15 ( 13 )	25 ( 24 )	3 ( 5 )	8 ( 8 )
625	133	204	15	11	47	61	10	28	5	11
	158 ( 146 )	183 ( 194 )	9 ( 12 )	15 ( 13 )	41 ( 44 )	63 ( 62 )	20 ( 15 )	18 ( 23 )	3 ( 4 )	6 ( 9 )
1250	151	167	11 *	13	47	62	21	20	6	8
	120 ( 136 )	162 ( 165 )	8 * ( 10 *)	10 ( 12 )	40 ( 44 )	64 ( 63 )	20 ( 21 )	14 ( 17 )	3 ( 5 )	10 ( 9 )
2500	0 *	169		13	0 *	57	0 *	21	0 *	6
	0 * ( 0 *)	153 ( 161 )		7 ( 10 )	0 * ( 0 *)	51 ( 54 )	0 * ( 0 *)	16 ( 19 )	0 * ( 0 *)	5 ( 6 )
5000	0 *	96 *		6 *	0 *	49 *	0 *	23 *	0 *	5 *
	0 * ( 0 *)	144 * ( 120 *)		5 * ( 6 *)	0 * ( 0 *)	44 * ( 47 *)	0 * ( 0 *)	10 * ( 17 *)	0 * ( 0 *)	6 * ( 6 *)
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive Control	AF-2 ( 673 )	2-AA ( 1115 )	NaN <sub>3</sub> ( 379 )	2-AA ( 279 )	AF-2 ( 580 )	2-AA ( 591 )	AF-2 ( 477 )	2-AA ( 430 )	9-AA ( 412 )	2-AA ( 138 )