

Chemical Name ; <u>2-Ethylhexanoic acid</u> Synonym ; <u>Hexanoic acid, 2-ethyl-</u> Molecular Weight ; 144.21 Melting Point ; - Boiling Point ; 228°C[Aldrich] Flashing Point ; >110°C[Aldrich] Molecular Formula ; C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> Chemical Structure $\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{C}_2\text{H}_5)\text{COOH}$ CAS No. ; 149-57-5 MITI No. ; (2)-608 ML No. ; - Specified Chemical Substances ; - Source of Substance; Tokyo Kasei Kogyo Co., Ltd. Lot No. ; FGE02 Purity ; >99% Vehicle ; DMSO	Conc. μ g/plate	Number of Revertants/plate									
		Base-substitution						Frame-shift			
		TA100		TA1535		WP2 <sub>uvrA/p</sub> KM101		TA98		TA1537	
		S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
	DMSO	( 128 )	( 137 )	( 7 )	( 12 )	( 41 )	( 53 )	( 17 )	( 29 )	( 6 )	( 6 )
		158	149	5	13	41	90	18	23	3	9
		139	156	6	10	43	70	16	29	5	6
	1 .22	( 149 )	( 153 )	( 6 )	( 12 )	( 42 )	( 80 )	( 17 )	( 26 )	( 4 )	( 8 )
		127	163	10	11	43	79	17	18	5	9
		113	136	8	8	52	59	16	26	6	7
	4 .88	( 120 )	( 150 )	( 9 )	( 10 )	( 48 )	( 69 )	( 17 )	( 22 )	( 6 )	( 8 )
		119	152	6	11	47	71	11	23	2	10
		148	126	6	7	39	71	25	30	5	6
19 .5	( 134 )	( 139 )	( 6 )	( 9 )	( 43 )	( 71 )	( 18 )	( 27 )	( 4 )	( 8 )	
	114	136	10	7	54	54	14	28	5	6	
	124	138	8	6	44	74	18	32	8	5	
78 .1	( 119 )	( 137 )	( 9 )	( 7 )	( 49 )	( 64 )	( 16 )	( 30 )	( 7 )	( 6 )	
	105	135	5	11	40	67	18	36	3	6	
	121	155	6	16	34	66	17	25	5	13	
313	( 113 )	( 145 )	( 6 )	( 14 )	( 37 )	( 67 )	( 18 )	( 31 )	( 4 )	( 10 )	
	116	153	8	9	37	61	16	23	3	15	
	120	108	8	10	49	56	11	29	5	7	
1250	( 118 )	( 131 )	( 8 )	( 10 )	( 43 )	( 59 )	( 14 )	( 26 )	( 4 )	( 11 )	
	75 *	85 *	3	6 *	32	28 *	8	7 *	3	2 *	
	68 *	70 *	7	0 *	21	33 *	8	14 *	5	5 *	
5000	( 72 *)	( 78 *)	( 5 )	( 3 *)	( 27 )	( 31 *)	( 8 )	( 11 *)	( 4 )	( 4 *)	
Judgement	-	-	-	-	-	-	-	-	-	-	
Specific Mutagenicity											
Positive Control	AF-2 ( 671 )	2-AA ( 1293 )	NaN <sub>3</sub> ( 456 )	2-AA ( 340 )	AF-2 ( 1301 )	2-AA ( 1056 )	AF-2 ( 553 )	2-AA ( 469 )	9-AA ( 741 )	2-AA ( 253 )	

\* Growth inhibition was observed.

Experimental Data-2

(B9706-2/2)

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+
	( 116 )	( 126 )	( 8 )	( 11 )	( 43 )	( 72 )	( 16 )	( 21 )	( 8 )	( 13 )
78 .1	130	141	6	9	37	61	20	23	7	17
	117 ( 124 )	141 ( 141 )	9 ( 8 )	11 ( 10 )	45 ( 41 )	79 ( 70 )	15 ( 18 )	30 ( 27 )	9 ( 8 )	11 ( 14 )
156	127	122	6	13	54	86	9	22	9	8
	123 ( 125 )	150 ( 136 )	6 ( 6 )	10 ( 12 )	57 ( 56 )	86 ( 86 )	21 ( 15 )	31 ( 27 )	11 ( 10 )	11 ( 10 )
313	135	111	3	13	61	56	11	18	8	11
	138 ( 137 )	143 ( 127 )	5 ( 4 )	10 ( 12 )	38 ( 50 )	71 ( 64 )	11 ( 11 )	23 ( 21 )	7 ( 8 )	13 ( 12 )
625	124	135	5	9	48	70	10	28	5	14
	124 ( 124 )	124 ( 130 )	7 ( 6 )	8 ( 9 )	48 ( 48 )	68 ( 69 )	11 ( 11 )	21 ( 25 )	9 ( 7 )	16 ( 15 )
1250	131	113	9	11	44	68	16	23	6	14
	102 ( 117 )	111 ( 112 )	6 ( 8 )	7 ( 9 )	40 ( 42 )	68 ( 68 )	16 ( 16 )	23 ( 23 )	6 ( 6 )	13 ( 14 )
2500	113	97	5	13	31	48	15	21	6	10
	101 ( 107 )	96 ( 97 )	3 ( 4 )	8 ( 11 )	38 ( 35 )	61 ( 55 )	18 ( 17 )	15 ( 18 )	11 ( 9 )	8 ( 9 )
5000	74 *	74 *	5	5 *	24	43 *	10	13 *	7	6 *
	77 * ( 76 * )	76 * ( 75 * )	5 ( 5 )	2 * ( 4 * )	25 ( 25 )	29 * ( 36 * )	11 ( 11 )	18 * ( 16 * )	7 ( 7 )	8 * ( 7 * )
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive Control	AF-2 ( 691 )	2-AA ( 1396 )	NaN <sub>3</sub> ( 469 )	2-AA ( 352 )	AF-2 ( 1541 )	2-AA ( 1160 )	AF-2 ( 636 )	2-AA ( 470 )	9-AA ( 643 )	2-AA ( 246 )