

Isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-diol

Experimental Data-1

(B9804-1/2)

(2,2,4-トリメチルペンタン-1,3-ジオールモノイソブチレート)

Chemical Name	: <u>Isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-diol</u>
Synonym	: <u>Propanoic acid, 2-methyl-, monoester with 2,2,4-trimethyl-1,3-pentanediol</u> イソ酪酸3-ヒドロキシ-2,2,4-トリメチルペンチル
Molecular Weight	: 216.32
Melting Point	: -50°C[Aldrich]
Boiling Point	: 244°C[Aldrich]
Flashing Point	: >110°C[Aldrich]
Molecular Formula	: C ₁₂ H ₂₄ O ₃
Chemical Structure	
CAS No.	: 25265-77-4
MITI No.	: (2)-778
ML No.	: -
Specified Chemical Substances	: -
Source of Substance	: Tokyo Kasei Kogyo Co., Ltd.
Lot No.	: GF01
Purity	: -
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+
		(122)	(117)	(12)	(12)	(63)	(85)	(19)	(26)	(7)
	149	133	2	11	49	98	13	22	3	13
0 .610	(144)	(123)	(9)	(9)	(64)	(84)	(15)	(22)	(7)	(6)
	117	133	7	15	45	99	20	21	6	8
2 .44	(130)	(149)	(10)	(17)	(63)	(100)	(22)	(29)	(3)	(5)
	106	114	8	13	62	108	22	34	3	9
9 .77	(158)	(117)	(9)	(10)	(69)	(82)	(16)	(30)	(3)	(9)
	149	133	14	8	61	100	20	15	2	10
39 .1	(146)	(151)	(13)	(10)	(69)	(68)	(15)	(31)	(10)	(6)
	131	142	8	14	54	74	22	28	5	6
156	(117)	(158)	(11)	(10)	(57)	(81)	(16)	(25)	(5)	(9)
	0 *	96 *	0 *	8 *	0 *	72 *	0 *	21 *	0 *	2 *
625	(0 *)	(108 *)	(0 *)	(8 *)	(0 *)	(60 *)	(0 *)	(29 *)	(0 *)	(5 *)
	0 *	0 *	0 *	0 *	0 *	0 *	0 *	0 *	0 *	0 *
2500	(0 *)	(0 *)	(0 *)	(0 *)	(0 *)	(0 *)	(0 *)	(0 *)	(0 *)	(0 *)
	0 *	0 *	0 *	0 *	0 *	0 *	0 *	0 *	0 *	0 *
10000	(0 *)	(0 *)	(0 *)	(0 *)	(0 *)	(0 *)	(0 *)	(0 *)	(0 *)	(0 *)
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive Control	AF-2 (557)	2-AA (1053)	NaN ₃ (426)	2-AA (256)	AF-2 (970)	2-AA (787)	AF-2 (504)	2-AA (418)	9-AA (514)	2-AA (178)

Mutagenicity in Bacterial Test ; Negative

IARC Evaluation ; not yet cited

* Growth inhibition was observed.

Experimental Data-2

(B9804-2/2)

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+
	(144)	(138)	(9)	(9)	(60)	(84)	(17)	(27)	(8)	(11)
9 .77	131	141	7	6	38	68	14	16	7	7
	116	155	5	5	40	84	18	15	5	5
19 .5	130	123	11	10	47	77	14	28	5	8
	127	150	3	11	68	99	16	23	3	13
39 .1	114	137	9	8	51	69	11	18	9	13
	133	123	6	7	44	108	10	11	5	8
78 .1	113	130	6	3	53	84	16	16	6	7
	142	136	7	10	72	93	20	17	7	5
156	117	128	5	11	60	74	10	14	5	10
	135	137	7	9	75	106	16	9	6	8
313	0 *	114	0 *	8	39 *	96	9 *	23	0 *	7
	0 *	130	0 *	9	30 *	91	8 *	15	0 *	9
625	0 *	76 *	0 *	6 *	0 *	67 *	0 *	16 *	0 *	7 *
	0 *	76 *	0 *	9 *	0 *	37 *	0 *	9 *	0 *	3 *
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive Control	AF-2 (671)	2-AA (1197)	NaN ₃ (445)	2-AA (241)	AF-2 (918)	2-AA (749)	AF-2 (485)	2-AA (476)	9-AA (489)	2-AA (147)