Chemical Name;Diisobutylene
Synonym ;Mixture of 2,4,4-Trimethyl-1-pentene and 2,4,4-Trimethyl-2-pentene (75:22)
2,4,4-ﾄﾘﾒﾁﾙ-1-ﾍﾟﾝﾃﾝと2,4,4--ﾄﾘﾒﾁﾙ-2-ﾍﾟﾝﾃﾝの混合物 (75:22)

① 2,4,4-Trimethyl-1-pentene
② 2,4,4-Trimethyl-2-pentene

Molecular Weight ; 112.21
Melting Point ; ① - 93.6 ℃ ② -106.3 ℃ [CHCD]
② -106 ℃ [Aldrich]
Boiling Point ; ① 101.2 ℃ ② 104.5 ℃ [CHCD]
① 101-102℃ ② 104 ℃ [Aldrich]
Flashing Point ; ① 2 ℃(o.c.) ② 2 ℃ [CHCD]
① - 6 ℃ ② -1 ℃ [Aldrich]
Molecular Formula; C_8H_{16}

Chemical Structure

① $(CH_3)_3CCH_2C(CH_3)=CH_2$

② $(CH_3)_3CCH=C(CH_3)_2$

CAS No. ; 25167-70-8
〔 ① 107-39-1 ② 107-40-4 〕
MITI No. ; (2)-24
ML No. ; —
Specified Chemical Substances; —

Source of Substance; Tokyo Kasei Kogyo Co.,Ltd.
Lot No. ; AQ01
Purity ; ① 75 % ② 22 %

Vehicle ; Acetone

Mutagenicity in Bacterial Test ; **Negative**

IARC Evaluation ; not yet cited

Conc. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2*uvrA*		TA98		TA1537	
	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+
Acetone	(126)	(129)	(8)	(7)	(28)	(34)	(12)	(23)	(6)	(12)
	153	135	10	6	25	31	10	20	2	6
	144	138	2	7	16	28	8	30	3	14
0.0763	(149)	(137)	(6)	(7)	(21)	(30)	(9)	(25)	(3)	(10)
	129	121	5	8	16	33	18	24	3	16
	138	119	15	8	22	28	17	28	8	9
0.305	(134)	(120)	(10)	(8)	(19)	(31)	(18)	(26)	(6)	(13)
	137	131	6	10	36	21	15	21	8	6
	121	142	11	8	16	26	11	22	2	13
1.22	(129)	(137)	(9)	(9)	(26)	(24)	(13)	(22)	(5)	(10)
	150	156	5	11	18	21	14	26	7	18
	124	128	8	8	25	24	14	25	8	11
4.88	(137)	(142)	(7)	(10)	(22)	(23)	(14)	(26)	(8)	(15)
	89*	126	7*	8	18*	29	10*	18	5*	13
	98*	129	3*	3	18*	21	14*	15	1*	13
19.5	(94*)	(128)	(5*)	(6)	(18*)	(25)	(12*)	(17)	(3*)	(13)
	0*	101	0*	8	0*	23	0*	17	0*	14
	0*	122	0*	7	0*	25	0*	24	0*	3
78.1	(0*)	(112)	(0*)	(8)	(0*)	(24)	(0*)	(21)	(0*)	(9)
	0*	0*	0*	0*	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*	0*	0*	0*	0*
313	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
	0*	0*	0*	0*	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*	0*	0*	0*	0*
1250	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
	0*	0*	0*	0*	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*	0*	0*	0*	0*
5000	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
Judgement	—	—	—	—	—	—	—	—	—	—
Specific Mutagenicity										
Positive Control	AF-2 (775)	2-AA (1262)	NaN_3 (378)	2-AA (255)	AF-2 (280)	2-AA (1071)	AF-2 (462)	2-AA (346)	9-AA (529)	2-AA (205)

Conc. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2*uvrA*		TA98		TA1537	
	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+
Acetone	(138)	(131)	(11)	(11)	(30)	(28)	(19)	(31)	(7)	(12)
	130		14		31		18		11	
	130		14		26		18		10	
0.305	(130)		(14)		(29)		(18)		(11)	
	144		13		26		14		10	
	133		5		36		20		7	
0.61	(139)		(9)		(31)		(17)		(9)	
	133		14		44		9		9	
	101		8		22		15		3	
1.22	(117)		(11)		(33)		(12)		(6)	
	120		10		26		30		7	
	136		3		28		17		2	
2.44	(128)		(7)		(27)		(24)		(5)	
	117	155	5	21	33	33	22	25	3	17
	138	128	11	13	24	30	17	29	5	11
4.88	(128)	(142)	(8)	(17)	(29)	(32)	(20)	(27)	(4)	(14)
	119	126	9	14	22	32	25	29	7	15
	144	133	5	10	40	30	16	25	5	14
9.77	(132)	(130)	(7)	(12)	(31)	(31)	(21)	(27)	(6)	(15)
	152*	145	5*	9	30*	29	13*	30	5*	11
	89*	128	5*	5	20*	38	14*	30	3*	11
19.5	(121*)	(137)	(5*)	(7)	(25*)	(34)	(14*)	(30)	(4*)	(11)
	115*	116	5*	8	18*	39	6*	36	5*	14
	94*	137	5*	8	25*	29	13*	25	6*	8
39.1	(105*)	(127)	(5*)	(8)	(22*)	(34)	(10*)	(31)	(6*)	(11)
		104		9		38		23		7
		90		6		45		24		14
78.1		(97)		(8)		(42)		(24)		(11)
		89*		11*		21*		17*		11*
		97*		6*		34*		18*		6*
156		(93*)		(9*)		(28*)		(18*)		(9*)
		0*		0*		0*		0*		0*
		0*		0*		0*		0*		0*
313		(0*)		(0*)		(0*)		(0*)		(0*)
Judgement	−	−	−	−	−	−	−	−	−	−
Specific Mutagenicity										
Positive Control	AF-2 (788)	2-AA (1257)	NaN_3 (363)	2-AA (297)	AF-2 (254)	2-AA (1199)	AF-2 (473)	2-AA (371)	9-AA (594)	2-AA (215)

Conc. μg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2*uvrA*/pKM101	
	S9−	S9+	S9−	S9+	S9−	S9+
Acetone	(218)	(296)	(258)	(342)	(44)	(69)
	238	267	313	356	37	83
	227	281	300	378	52	52
0.0191	(233)	(274)	(307)	(367)	(45)	(68)
	249	271	317	366	45	56
	218	297	322	343	34	56
0.0763	(234)	(284)	(320)	(355)	(40)	(56)
	222	306	311	347	40	60
	229	285	373	342	48	68
0.305	(226)	(296)	(342)	(345)	(44)	(64)
	218	286	334	373	41	59
	213	311	332	334	51	60
1.22	(216)	(299)	(333)	(354)	(46)	(60)
	238	307	299	343	43	75
	219	290	309	374	40	59
4.88	(229)	(299)	(304)	(359)	(42)	(67)
	212	299	311	322	36*	67
	187	279	293	361	38*	56
19.5	(200)	(289)	(302)	(342)	(37*)	(62)
	0*	269*	0*	266*	0*	81
	0*	301*	0*	338*	0*	61
78.1	(0*)	(285*)	(0*)	(302*)	(0*)	(71)
	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*
313	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*
1250	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*
5000	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
Judgement	−	−	−	−	−	−
Specific Mutagenicity						
Positive Control	BLM (735)	2-AA (2645)	PA (1363)	2-AA (1049)	AF-2 (1155)	2-AA (974)

Conc. μg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2*uvrA*/pKM101	
	S9−	S9+	S9−	S9+	S9−	S9+
Acetone	(226)	(326)	(323)	(354)	(36)	(53)
					33	
					40	
0.305					(37)	
					47	
					44	
0.61					(46)	
	267	343	331	329	47	
	273	349	312	355	44	
1.22	(270)	(346)	(322)	(342)	(46)	
	263	340	335	396	41	
	272	313	348	378	41	
2.44	(268)	(327)	(342)	(387)	(41)	
	255	334	305	388	51	66
	265	300	268	356	44	69
4.88	(260)	(317)	(287)	(372)	(48)	(68)
	255	326	291	352	36	75
	242	323	340	368	30	77
9.77	(249)	(325)	(316)	(360)	(33)	(76)
	150	324	313*	337	26*	49
	202	298	258*	372	24*	77
19.5	(176)	(311)	(286*)	(355)	(25*)	(63)
	0*	295	325*	332		55
	0*	280	280*	331		61
39.1	(0*)	(288)	(303*)	(332)		(58)
	0*	306*	290*	285*		49*
	0*	239*	290*	318*		82*
78.1	(0*)	(273*)	(290*)	(302*)		(66*)
						0*
						0*
156						(0*)
						0*
						0*
313						(0*)
Judgement	−	−	−	−	−	−
Specific Mutagenicity						
Positive Control	BLM (742)	2-AA (4513)	PA (1539)	2-AA (1231)	AF-2 (1424)	2-AA (992)

Experimental Data - 5

Conc. μg/plate	Number of Revertants/plate Base-substitution TA102 S9−	S9+
Acetone	280 297 (289)	(345)
1.22	272 279 (276)	343 358 (351)
2.44	291 285 (288)	346 348 (347)
4.88	258 292 (275)	316 331 (324)
9.77	157 263 (210)	349 365 (357)
19.5	0* 0* (0*)	372 347 (360)
39.1		313* 286* (300*)
78.1		
Judgement	−	−
Specific Mutagenicity		
Positive Control	BLM (693)	2-AA (1207)