

Pentaerythritol

[ペンタエリトリール]

Experimental Data - 1

(B9512-1/3)

Chemical Name; Pentaerythritol
 Synonym ; 2,2-Bis(hydroxymethyl)-1,3-propane diol
Tetrakis(hydroxymethyl)methane
2,2-ビス(ヒドロキシメチル)-1,3-プロパンジオール
テトラキス(ヒドロキシメチル)メタン

Molecular Weight ; 136.15
 Melting Point ; 260 ℃ [CHCD;Merck]
 255 - 259 ℃ [Aldrich]
 Boiling Point ; - ℃
 Flashing Point ; - ℃
 Molecular Formula; C₅H₁₂O₄

Chemical Structure

$$\begin{array}{c}
 \text{CH}_2\text{OH} \\
 | \\
 \text{HOH}_2\text{C}-\text{C}-\text{CH}_2\text{OH} \\
 | \\
 \text{CH}_2\text{OH}
 \end{array}$$

CAS No. ; 115-77-5
 MITI No. ; (2)-248
 ML No. ; -
 Specified Chemical Substances; -

Source of Substance; Tokyo Kasei Kogyo Co.,Ltd.
 Lot No. ; GC01
 Purity ; 99.6 %

Vehicle ; DMSO

Conc. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA		TA98		TA1537	
	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
DMSO	(122)	(122)	(10)	(9)	(25)	(29)	(21)	(34)	(12)	(14)
	117	112	5	10	31	25	18	24	7	9
	129	109	7	7	18	41	25	32	10	14
0.0763	(123)	(111)	(6)	(9)	(25)	(33)	(22)	(28)	(9)	(12)
	116	111	9	8	25	17	13	38	10	13
	109	107	7	8	28	34	17	16	10	15
0.305	(113)	(109)	(8)	(8)	(27)	(26)	(15)	(27)	(10)	(14)
	127	128	5	14	26	20	10	25	10	16
	127	101	5	11	23	31	9	20	8	14
1.22	(127)	(115)	(5)	(13)	(25)	(26)	(10)	(23)	(9)	(15)
	109	129	5	13	30	26	22	23	8	18
	89	106	13	7	16	26	13	31	20	9
4.88	(99)	(118)	(9)	(10)	(23)	(26)	(18)	(27)	(14)	(14)
	89	135	1	11	26	28	24	28	7	15
	105	109	3	5	28	33	20	24	10	18
19.5	(97)	(122)	(2)	(8)	(27)	(31)	(22)	(26)	(9)	(17)
	111	107	3	11	17	24	14	31	6	10
	120	126	9	8	17	28	18	30	14	14
78.1	(116)	(117)	(6)	(10)	(17)	(26)	(16)	(31)	(10)	(12)
	114	102	11	8	26	34	16	34	6	9
	122	113	15	6	31	21	21	40	8	11
313	(118)	(108)	(13)	(7)	(29)	(28)	(19)	(37)	(7)	(10)
	112	115	6	9	28	29	18	31	7	13
	135	112	7	11	13	30	22	20	10	11
1250	(124)	(114)	(7)	(10)	(21)	(30)	(20)	(26)	(9)	(12)
	111	106	10	11	22	22	15	23	7	18
	108	122	10	11	21	20	18	31	16	15
5000	(110)	(114)	(10)	(11)	(22)	(21)	(17)	(27)	(12)	(17)
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive Control	AF-2 (934)	2-AA (1457)	NaN ₃ (334)	2-AA (285)	AF-2 (492)	2-AA (1020)	AF-2 (277)	2-AA (419)	9-AA (534)	2-AA (215)

Mutagenicity in Bacterial Test ; **Negative**

IARC Evaluation ; not yet cited

Experimental Data - 2

Conc. µg/plate	Number of Revertants/plate	
	Base-substitution	
	WP2uvrA	
	S9-	S9+
DMSO	(38)	(43)
	40	45
	43	40
313	(42)	(43)
	48	38
	34	41
625	(41)	(40)
	38	46
	43	30
1250	(41)	(38)
	44	48
	47	32
2500	(46)	(40)
	37	37
	32	31
5000	(35)	(34)

Judgement	-	-
Specific Mutagenicity		
Positive	AF-2	2-AA
Control	(190)	(1154)

Experimental Data - 3

(B9512-2/3)

Conc. µg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA		TA98		TA1537	
	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
DMSO	(128)	(137)	(9)	(11)	(22)	(26)	(17)	(20)	(6)	(8)
	127	131	10	9	26	25	28	21	2	8
	137	143	13	6	22	41	18	13	3	10
313	(132)	(137)	(12)	(8)	(24)	(33)	(23)	(17)	(3)	(9)
	129	145	9	9	20	20	24	39	3	5
	122	137	3	13	18	26	23	29	7	10
625	(126)	(141)	(6)	(11)	(19)	(23)	(24)	(34)	(5)	(8)
	128	134	10	13	18	26	21	28	5	10
	126	143	7	6	24	25	15	26	1	3
1250	(127)	(139)	(9)	(10)	(21)	(26)	(18)	(27)	(3)	(7)
	131	148	7	14	31	25	6	23	5	7
	123	143	11	9	21	21	21	28	7	8
2500	(127)	(146)	(9)	(12)	(26)	(23)	(14)	(26)	(6)	(8)
	144	130	7	13	21	32	13	30	6	7
	124	123	6	6	30	31	13	21	1	6
5000	(134)	(127)	(7)	(10)	(26)	(32)	(13)	(26)	(4)	(7)

Judgement	-	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity											
Positive	AF-2	2-AA	NaN ₃	2-AA	AF-2	2-AA	AF-2	2-AA	9-AA	2-AA	
Control	(849)	(1250)	(431)	(277)	(299)	(1128)	(404)	(445)	(613)	(203)	

Experimental Data - 4

Conc. µg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2uvrA/pKM101	
	S9-	S9+	S9-	S9+	S9-	S9+
DMSO	(230)	(287)	(270)	(350)	(49)	(63)
	219	304	276	362	45	69
	227	275	282	365	48	66
4.88	(223)	(290)	(279)	(364)	(47)	(68)
	216	303	324	337	55	60
	227	320	262	368	49	72
19.5	(222)	(312)	(293)	(353)	(52)	(66)
	248	298	317	371	46	68
	261	272	299	340	48	68
78.1	(255)	(285)	(308)	(356)	(47)	(68)
	246	297	268	377	43	70
	255	271	291	355	66	59
313	(251)	(284)	(280)	(366)	(55)	(65)
	206	324	316	334	49	90
	228	275	310	355	49	67
1250	(217)	(300)	(313)	(345)	(49)	(79)
	271	311	281	356	47	60
	214	243	278	306	36	72
5000	(243)	(277)	(280)	(331)	(42)	(66)
Judgement	—	—	—	—	—	—
Specific Mutagenicity						
Positive Control	BLM (644)	2-AA (3230)	PA (1683)	2-AA (1163)	AF-2 (1009)	2-AA (827)

Experimental Data - 5

(B9512-3/3)

Conc. µg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2uvrA/pKM101	
	S9-	S9+	S9-	S9+	S9-	S9+
DMSO	(232)	(277)	(292)	(378)	(42)	(64)
	226	314	285	358	38	70
	236	309	324	364	45	53
313	(231)	(312)	(305)	(361)	(42)	(62)
	271	323	303	372	38	68
	254	328	290	376	43	57
625	(263)	(326)	(297)	(374)	(41)	(63)
	274	303	278	355	33	53
	218	303	326	404	33	60
1250	(246)	(303)	(302)	(380)	(33)	(57)
	276	313	295	396	44	70
	234	292	336	412	36	67
2500	(255)	(303)	(316)	(404)	(40)	(69)
	227	292	319	353	44	67
	259	293	304	305	38	56
5000	(243)	(293)	(312)	(329)	(41)	(62)
Judgement	—	—	—	—	—	—
Specific Mutagenicity						
Positive Control	BLM (523)	2-AA (1629)	PA (1259)	2-AA (1023)	AF-2 (1028)	2-AA (756)