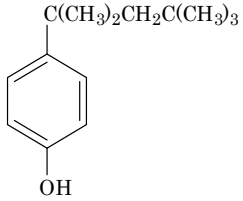
Chemical Name ; 4-(1,1,3,3,-Tetramethylbutyl) phenol

Synonym ; 4-*tert*-Octylphenol
p-*tert*-Octylphenol
p-*tert*-オクチルフェノール

Molecular Weight ; 206.33
Melting Point ; 81-84℃[Aldrich]
Boiling Point ; 290 ℃[CHCD]
Flashing Point ; −
Molecular Formula ; $C_{14}H_{22}O$

Chemical Structure



CAS No. ; 140-66-9
MITI No. ; (3)-503
ML No. ; −
Specified Chemical Substances ; −

Source of Substance; Tokyo Kasei Kogyo Co., Ltd.
Lot No. ; GC01
Purity ; 93%

Vehicle ; DMSO

Mutagenicity in Bacterial Test ; Negative

IARC Evaluation ; not yet cited

Conc. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2*uvr*A		TA98		TA1537	
	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+
DMSO	(158)	(155)	(8)	(12)	(18)	(24)	(13)	(20)	(5)	(7)
1 .22	117 130 (124)	144 190 (167)	5 8 (7)	10 8 (9)	14 20 (17)	25 11 (18)	18 11 (15)	17 25 (21)	5 2 (4)	3 6 (5)
4 .88	127 148 (138)	216 225 (221)	5 7 (6)	5 11 (8)	17 11 (14)	22 20 (21)	20 13 (17)	24 31 (28)	2 5 (4)	6 7 (7)
19 .5	0 * 0 * (0 *)	230 216 (223)	0 * 0 * (0 *)	3 7 (5)	7 15 (11)	30 32 (31)	0 * 0 * (0 *)	22 29 (26)	0 * 0 * (0 *)	6 6 (6)
78 .1	0 * 0 * (0 *)	166 * 151 * (159 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	6 * 7 * (7 *)	18 15 (17)	0 * 0 * (0 *)	17 * 21 * (19 *)	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 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)	0 * 0 * (0 *)
Judgement	−	−	−	−	−	−	−	−	−	−
Specific Mutagenicity										
Positive Control	AF-2 (681)	2-AA (1271)	NaN_3 (292)	2-AA (233)	AF-2 (323)	2-AA (1053)	AF-2 (364)	2-AA (445)	9-AA (763)	2-AA (175)

* Growth inhibitation was observed.
† Test chemical was precipitated with and without S9mix.

Conc. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2*uvr*A		TA98		TA1537	
	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+
DMSO	(155)	(164)	(7)	(8)	(21)	(22)	(13)	(22)	(8)	(10)
	157		5				15		7	
	181		7				14		6	
0 .610	(169)		(6)				(15)		(7)	
	158		5				11		7	
	172		9				17		6	
1 .22	(165)		(7)				(14)		(7)	
	165	233	6	6	15		16	22	6	11
	162	238	8	9	14		13	22	3	6
2 .44	(164)	(236)	(7)	(8)	(15)		(15)	(22)	(5)	(9)
	119	211	5	10	13		18	18	7	9
	149	208	8	9	24		17	25	6	10
4 .88	(134)	(210)	(7)	(10)	(19)		(18)	(22)	(7)	(10)
	122 *	233	0 *	11	11	31	0 *	24	0 *	10
	142 *	230	0 *	9	23	26	0 *	21	0 *	7
9 .77	(132 *)	(232)	(0 *)	(10)	(17)	(29)	(0 *)	(23)	(0 *)	(9)
	0 *	249	0 *	7	16	28	0 *	18	0 *	5
	0 *	218	0 *	6	17	28	0 *	23	0 *	8
19 .5	(0 *)	(234)	(0 *)	(7)	(17)	(28)	(0 *)	(21)	(0 *)	(7)
		200 *		9 *	8 *	17		23 *		8 *
		186 *		2 *	9 *	22		25 *		3 *
39 .1		(193 *)		(6 *)	(9 *)	(20)		(24 *)		(6 *)
		160 *		0 *	8 *	21		17 *		0 *
		143 *		0 *	7 *	17		22 *		0 *
78 .1		(152 *)		(0 *)	(8 *)	(19)		(20 *)		(0 *)
						15 *				
						14 *				
156						(15 *)				
						0 *				
						0 *				
313						(0 *)				
Judgement	−	−	−	−	−	−	−	−	−	−
Specific Mutagenicity										
Positive Control	AF-2 (734)	2-AA (1256)	NaN_3 (283)	2-AA (222)	AF-2 (249)	2-AA (1053)	AF-2 (485)	2-AA (479)	9-AA (873)	2-AA (170)

Conc. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2*uvr*A		TA98		TA1537	
	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+
DMSO	(133)	(152)	(8)	(10)	(24)	( )	(15)	(24)	(6)	(10)
	152		3				16		3	
	130		6				15		7	
0 .305	(141)		(5)				(16)		(5)	
	122		7				16		7	
	127		7				14		3	
0 .610	(125)		(7)				(15)		(5)	
	130	188	6	8	26		15	24	6	8
	129	185	3	9	11		13	22	6	5
1 .22	(130)	(187)	(5)	(9)	(19)		(14)	(23)	(6)	(7)
	133	171	6	8	11		13	25	5	9
	127	159	13	11	25		11	29	5	6
2 .44	(130)	(165)	(10)	(10)	(18)		(12)	(27)	(5)	(8)
	111	192	10	5	30		20	18	6	6
	127	180	9	9	17		8	29	3	10
4 .88	(119)	(186)	(10)	(7)	(24)		(14)	(24)	(5)	(8)
	111 *	149	0 *	14	28		0 *	24	0 *	10
	94 *	186	0 *	9	29		0 *	28	0 *	14
9 .77	(103 *)	(168)	(0 *)	(12)	(29)		(0 *)	(26)	(0 *)	(12)
		144		7	17			30		6
		169		8	18			26		6
19 .5		(157)		(8)	(18)			(28)		(6)
		150 *		6 *	13 *			14 *		8 *
		150 *		7 *	15 *			24 *		10 *
39 .1		(150 *)		(7 *)	(14 *)			(19 *)		(9 *)
Judgement	−	−	−	−	−		−	−	−	−
Specific Mutagenicity										
Positive Control	AF-2 (593)	2-AA (872)	NaN_3 (328)	2-AA (235)	AF-2 (231)		AF-2 (471)	2-AA (462)	9-AA (852)	2-AA (202)

Experimental Data-4

Conc. μg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2*uvr*A/pKM101	
	S9−	S9+	S9−	S9+	S9−	S9+
DMSO	(306)	(361)	(314)	(376)	(43)	(57)
	348	380	282	356	39	61
	329	385	293	353	53	56
0 .0763	(339)	(383)	(288)	(355)	(46)	(59)
	316	380	348	349	43	68
	299	400	290	390	28	70
0 .305	(308)	(390)	(319)	(370)	(36)	(69)
	326	404	306	360	38	87
	337	412	305	435	36	46
1 .22	(332)	(408)	(306)	(398)	(37)	(67)
	338	422	313	395	39	55
	325	460	298	410	44	46
4 .88	(332)	(441)	(306)	(403)	(42)	(51)
	136 *	450	253 *	393	29 *	72
	163 *	440	221 *	407	23 *	74
19 .5	(150 *)	(445)	(237 *)	(400)	(26 *)	(73)
	0 *	358	0 *	350 *	0 *	43 *
	0 *	358	0 *	325 *	0 *	57 *
78 .1	(0 *)	(358)	(0 *)	(338 *)	(0 *)	(50 *)
	0 *	78 *	0 *	123 *	0 *	0 *
	0 *	72 *	0 *	81 *	0 *	0 *
313	(0 *)	(75 *)	(0 *)	(102 *)	(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 (891)	2-AA (1250)	PA (1652)	2-AA (1280)	AF-2 (1938)	2-AA (1140)

Experimental Data-5 (B9624-4/4)

Conc. μg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2*uvr*A/pKM101	
	S9−	S9+	S9−	S9+	S9−	S9+
DMSO	(278)	(348)	(244)	(281)	(47)	(79)
	272		233		66	
	271		243		54	
0 .610	(272)		(238)		(60)	
	312		287		56	
	279		252		52	
1 .22	(296)		(270)		(54)	
	294		271	382	38	72
	287		249	364	48	86
2 .44	(291)		(260)	(373)	(43)	(79)
	238		263	361	48	61
	260		243	328	59	71
4 .88	(249)		(253)	(345)	(54)	(66)
	192	346	209	368	39	81
	202	365	218	341	46	82
9 .77	(197)	(356)	(214)	(355)	(43)	(82)
	134	371	176	310	28	90
	157	395	178	319	26	90
19 .5	(146)	(383)	(177)	(315)	(27)	(90)
		372		303		68
		348		328		68
39 .1		(360)		(316)		(68)
		297		311		70
		278		288		59
78 .1		(288)		(300)		(65)
		185				
		211				
156		(198)				
		36				
		70				
313		(53)				
Judgement	−	−	−	−	−	−
Specific Mutagenicity						
Positive Control	BLM (737)	2-AA (933)	PA (1593)	2-AA (1502)	AF-2 (1483)	2-AA (939)