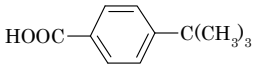
p-tert-Butylbenzoic acid (*p*-tert-ブチル安息香酸)

Chemical Name ; *p*-tert-Butylbenzoic acid
Synoym ; 4-*tert*-Butylbenzoic acid
4-(1,1-Dimethylethyl)benzoic acid
Molecular Weight ; 178.23
Melting Point ; 163-164.4℃[CHCD]
Boiling Point ; −
Flashing Point ; −
Molecular Formular; $C_{11}H_{14}O_2$

Chemical Structure;



CAS No. ; 98-73-7
METI No. ; (3)-1338
MHLW No. ; −
Specified Chemical Substances; −

Source of Substance; Tokyo Kasei Kogyo Co., Ltd.
Lot No. ; GA05
Purity ; >99%

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*uvrA*/pKM101		TA98		TA1537	
	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+
DMSO	(106)	(125)	(12)	(9)	(70)	(100)	(15)	(26)	(9)	(11)
	106	122	5	11	45	77	7	29	10	3
	97	107	7	10	53	114	22	33	7	13
1 .22	(102)	(115)	(6)	(11)	(49)	(96)	(15)	(31)	(9)	(8)
	119	134	6	7	70	84	15	23	5	11
	99	115	9	9	81	92	18	25	13	9
4 .88	(109)	(125)	(8)	(8)	(76)	(88)	(17)	(24)	(9)	(10)
	86	134	7	7	59	108	17	18	5	10
	104	102	14	10	63	85	10	17	5	9
19 .5	(95)	(118)	(11)	(9)	(61)	(97)	(14)	(18)	(5)	(10)
	99	97	7	13	67	100	13	25	3	5
	91	108	7	6	60	87	9	29	8	10
78 .1	(95)	(103)	(7)	(10)	(64)	(94)	(11)	(27)	(6)	(8)
	99	120	9	5	63	116	8	18	6	11
	90	98	14	6	61	84	13	23	9	13
313	(95)	(109)	(12)	(6)	(62)	(100)	(11)	(21)	(8)	(12)
	69	89	6	6	71	66	13	15	5	6
	72	90	10	8	78	79	7	16	11	3
1250	(71)	(90)	(8)	(7)	(75)	(73)	(10)	(16)	(8)	(5)
	24 *	32 *	0 *	6 *	38 *	40 *	3 *	13 *	3 *	0 *
	28 *	38 *	2 *	6 *	21 *	26 *	15 *	9 *	2 *	3 *
5000	(26 *)	(35 *)	(1 *)	(6 *)	(30 *)	(33 *)	(9 *)	(11 *)	(3 *)	(2 *)
Judgement	−	−	−	−	−	−	−	−	−	−
Specific Mutagenicity										
Positive Control	AF-2 (641)	2-AA (1255)	NaN_3 (443)	2-AA (266)	AF-2 (1011)	2-AA (913)	AF-2 (482)	2-AA (469)	9-AA (463)	2-AA (260)

* Growth inhibition was observed.

Conc. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2*uvrA*/pKM101		TA98		TA1537	
	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+
DMSO	(103)	(126)	(10)	(9)	(70)	(97)	(16)	(24)	(10)	(13)
	119	152	16	9	60	100	11	23	14	20
	105	113	3	5	61	91	15	18	11	16
156	(112)	(133)	(10)	(7)	(61)	(96)	(13)	(21)	(13)	(18)
	112	138	7	5	87	106	25	17	21	10
	84	106	14	10	76	127	17	23	8	10
313	(98)	(122)	(11)	(8)	(82)	(117)	(21)	(20)	(15)	(10)
	96	105	7	10	75	96	9	21	9	17
	112	93	9	10	70	117	16	20	15	7
625	(104)	(99)	(8)	(10)	(73)	(107)	(13)	(21)	(12)	(12)
	78	98	6	5	81	70	8	28	5	13
	83	74	9	6	83	89	9	10	11	10
1250	(81)	(86)	(8)	(6)	(82)	(80)	(9)	(19)	(8)	(12)
	74	71 *	8	5 *	78	84	16 *	28 *	5	1 *
	76	54 *	3	11 *	66	78	16 *	11 *	5	0 *
2500	(75)	(63 *)	(6)	(8 *)	(72)	(81)	(16 *)	(20 *)	(5)	(1 *)
	23 *	43 *	5 *	3 *	66 *	31 *	8 *	14 *	5 *	1 *
	16 *	31 *	6 *	3 *	37 *	25 *	7 *	9 *	6 *	2 *
5000	(20 *)	(37 *)	(6 *)	(3 *)	(52 *)	(28 *)	(8 *)	(12 *)	(6 *)	(2 *)
Judgement	−	−	−	−	−	−	−	−	−	−
Specific Mutagenicity										
Positive Control	AF-2 (802)	2-AA (1561)	NaN_3 (451)	2-AA (254)	AF-2 (938)	2-AA (987)	AF-2 (487)	2-AA (418)	9-AA (322)	2-AA (245)

* Growth inhibition was observed.