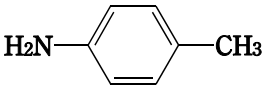
Chemical Name; *p*-Toluidine
Synonym ; 4-Methylaniline
4-Methylbenzenamine
4-Aminotoluene
p-Tolylamine
4-メチルアニリン
4-メチルベンゼナミン
4-アミノトルエン
p-トリルアミン

Molecular Weight ; 107.16
Melting Point ; 45 ℃ [CHCD]
41 - 46 ℃ [Aldrich]
44 - 45 ℃ [Merck]
Boiling Point ; 82.2 ℃(10mmHg) [CHCD]
200 ℃ [Aldrich]
200 - 201 ℃ [Merck]
Flashing Point ; 88 ℃ [Aldrich]
86 ℃ (c.c.) [Merck]
Molecular Formula; C_7H_9N

Chemical Structure



CAS No. ; 95-53-4
MITI No. ; (3)-186
ML No. ; —
Specified Chemical Substances; —

Source of Substance; Tokyo Kasei Kogyo Co.,Ltd.
Lot No. ; FHC01
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*		TA98		TA1537	
	S9－	Ham.S9＋	S9－	Ham.S9＋	S9－	Ham.S9＋	S9－	Ham.S9＋	S9－	Ham.S9＋
DMSO	(106)	(133)	(7)	(11)	(26)	(32)	(18)	(30)	(5)	(7)
	120	143	9	11	23	36	23	41	9	5
	119	138	7	3	25	21	17	36	5	5
0.0763	(120)	(141)	(8)	(7)	(24)	(29)	(20)	(39)	(7)	(5)
	109	152	8	5	23	25	21	29	11	6
	111	144	11	6	17	26	24	33	5	7
0.305	(110)	(148)	(10)	(6)	(20)	(26)	(23)	(31)	(8)	(7)
	97	127	6	11	22	32	20	22	3	6
	112	158	6	9	18	30	28	33	3	1
1.22	(105)	(143)	(6)	(10)	(20)	(31)	(24)	(28)	(3)	(4)
	150	127	3	16	24	21	20	33	2	3
	106	164	3	14	31	32	20	26	7	6
4.88	(128)	(146)	(3)	(15)	(28)	(27)	(20)	(30)	(5)	(5)
	108	152	8	10	25	28	28	26	2	6
	99	166	7	7	20	37	20	21	2	7
19.5	(104)	(159)	(8)	(9)	(23)	(33)	(24)	(24)	(2)	(7)
	107	169	8	7	20	25	24	49	6	5
	105	146	9	10	29	31	20	26	5	2
78.1	(106)	(158)	(9)	(9)	(25)	(28)	(22)	(38)	(6)	(4)
	108	169	5	11	22	28	21	28	2	6
	99	188	8	8	10	23	20	26	6	1
313	(104)	(179)	(7)	(10)	(16)	(26)	(21)	(27)	(4)	(4)
	136	211	5	8	20	34	16	36	3	10
	112	197	7	9	22	34	13	23	8	9
1250	(124)	(204)	(6)	(9)	(21)	(34)	(15)	(30)	(6)	(10)
	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 (707)	2-AA (3139)	NaN_3 (341)	2-AA (542)	AF-2 (221)	2-AA (1381)	AF-2 (487)	2-AA (956)	9-AA (702)	2-AA (627)

※ Ham.S9 : Hamster S9

Conc. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2*uvrA*		TA98		TA1537	
	S9－	Ham.S9＋	S9－	Ham.S9＋	S9－	Ham.S9＋	S9－	Ham.S9＋	S9－	Ham.S9＋
DMSO	(112)	(142)	(11)	(9)	(20)	(20)	(15)	(22)	(6)	(5)
	114	149	11	13	8	23	16	24	1	3
	106	158	8	13	16	15	17	24	1	8
78.1	(110)	(154)	(10)	(13)	(12)	(19)	(17)	(24)	(1)	(6)
	114	151	11	20	17	32	13	32	5	2
	114	156	1	14	17	28	6	20	3	6
156	(114)	(154)	(6)	(17)	(17)	(30)	(10)	(26)	(4)	(4)
	121	163	6	9	20	20	16	23	3	3
	128	186	2	6	14	26	11	31	3	6
313	(125)	(175)	(4)	(8)	(17)	(23)	(14)	(27)	(3)	(5)
	122	176	5	15	9	18	15	29	2	5
	109	195	13	13	26	21	14	28	7	7
625	(116)	(186)	(9)	(14)	(18)	(20)	(15)	(29)	(5)	(6)
	120	199	8	2	20	24	18	23	6	5
	107	198	16	10	20	20	14	31	8	8
1250	(114)	(199)	(12)	(6)	(20)	(22)	(16)	(27)	(7)	(7)
	105*	164*	1*	7*	18	16	11*	16*	1*	8*
	86*	159*	13*	8*	16	23	9*	30*	3*	5*
2500	(96*)	(162*)	(7*)	(8*)	(17)	(20)	(10*)	(23*)	(2*)	(7*)
	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 (863)	2-AA (3890)	NaN_3 (311)	2-AA (446)	AF-2 (371)	2-AA (1433)	AF-2 (413)	2-AA (1126)	9-AA (667)	2-AA (713)

※ Ham.S9 : Hamster S9

Experimental Data - 3

Conc. μg/plate	Number of Revertants/plate Base-substitution TA102 S9−	TA102 Ham.S9+	TA104 S9−	TA104 Ham.S9+	WP2*uvrA*/pKM101 S9−	WP2*uvrA*/pKM101 Ham.S9+
DMSO	(277)	(374)	(349)	(454)	(39)	(72)
	233	347	312	427	36	60
	241	362	299	412	25	76
0.0763	(237)	(355)	(306)	(420)	(31)	(68)
	274	343	324	425	60	67
	242	366	367	407	46	67
0.305	(258)	(355)	(346)	(416)	(53)	(67)
	276	365	306	441	45	68
	252	324	348	402	51	62
1.22	(264)	(345)	(327)	(422)	(48)	(65)
	273	323	334	450	39	72
	255	335	313	417	54	84
4.88	(264)	(329)	(324)	(434)	(47)	(78)
	255	352	343	417	51	60
	265	340	344	399	57	82
19.5	(260)	(346)	(344)	(408)	(54)	(71)
	267	331	362	444	45	92
	269	349	329	438	41	87
78.1	(268)	(340)	(346)	(441)	(43)	(90)
	241	322	359	488	52	90
	265	356	365	417	51	90
313	(253)	(339)	(362)	(453)	(52)	(90)
	291*	294	380*	471	59	86
	278*	324	320*	498	69	81
1250	(285*)	(309)	(350*)	(485)	(64)	(84)
	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 (867)	2-AA (1809)	PA (1583)	2-AA (2123)	AF-2 (1040)	2-AA (1495)

※ Ham.S9 : Hamster S9

Experimental Data - 4

(B9517-3/3)

Conc. μg/plate	Number of Revertants/plate Base-substitution TA102 S9−	TA102 Ham.S9+	TA104 S9−	TA104 Ham.S9+	WP2*uvrA*/pKM101 S9−	WP2*uvrA*/pKM101 Ham.S9+
DMSO	(259)	(339)	(310)	(364)	(37)	(58)
	222		284			
	241		294			
19.5	(232)		(289)			
	212		286			
	216		282			
39.1	(214)		(284)			
	247	320	281	387	18	53
	214	320	262	358	32	56
78.1	(231)	(320)	(272)	(373)	(25)	(55)
	225	328	306	366	38	71
	240	340	281	410	28	68
156	(233)	(334)	(294)	(388)	(33)	(70)
	243	313	243	361	34	63
	240	295	301	385	32	69
313	(242)	(304)	(272)	(373)	(33)	(66)
	227*	313	274*	457	53	81
	234*	342	275*	404	41	64
625	(231*)	(328)	(275*)	(431)	(47)	(73)
	262*	331	297*	382	34	60
	218*	312	273*	441	45	67
1250	(240*)	(322)	(285*)	(412)	(40)	(64)
	236*	306*	267*	401*	38*	61*
	229*	273*	248*	370*	40*	53*
2500	(233*)	(290*)	(258*)	(386*)	(39*)	(57*)
		0*		0*	0*	0*
		0*		0*	0*	0*
5000		(0*)		(0*)	(0*)	(0*)
Judgement	−	−	−	−	−	−
Specific Mutagenicity						
Positive Control	BLM (743)	2-AA (1499)	PA (1480)	2-AA (1931)	AF-2 (1382)	2-AA (1636)

※ Ham.S9 : Hamster S9