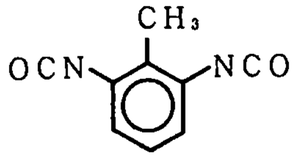
Toluene 2,6-diisocyanate (トルエン 2,6-ジイソシアナート)

Chemical Name: Toluene 2,6-diisocyanate
Synonym Benzene, 1,3-diisocyanato-2-methyl-
Molecular weight: 174.15
Boiling point: 129～133℃(18mmHg)

Chemical Structure



CAS No : 91-08-7
MITI No: (3)-2214
Specified chemical substamces: G2
Source of Substance: Tokyo Kasei Kogyo Co., Ltd.
Lot.No.: AW01
Purity: 95 %
Vehicle: DSMO

Mutagenicity in Bacterial Test: Positive

IARC Evaluation: G 2 B

Experimental Data

Con. 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+
DSMO	(132)	(145)	(9)	(10)	(20)	(25)	(20)	(22)	(7)	(13)
	145	171	8	8	17	23	21	32	5	11
	142	172	8	14	17	15	23	30	7	13
20	(144)	(172)	(8)	(11)	(17)	(19)	(22)	(31)	(6)	(12)
	153	223	16	13	15	22	10	46	2	9
	144	183	11	7	21	30	22	44	8	13
39	(149)	(203)	(14)	(10)	(18)	(26)	(16)	(45)	(5)	(11)
	162	238	10	11	24	17	20	37	9	3
	158	218	10	10	17	33	17	45	17	10
78	(160)	(228)	(10)	(11)	(21)	(25)	(19)	(41)	(13)	(7)
	156	248	8	7	21	20	18	48	5	5
	134	201	11	11	24	28	16	39	7	9
156	(145)	(225)	(10)	(9)	(23)	(24)	(17)	(44)	(6)	(7)
	127	215	9	14	21	32	22	39	9	10
	139	253	5	7	17	31	22	49	11	10
313	(133)	(234)	(7)	(11)	(19)	(32)	(22)	(44)	(10)	(10)
	141	178	8	11	15	24	15	39	4	7
	126	174	4	6	20	18	12	41	5	15
625	(134)	(176)	(6)	(9)	(18)	(21)	(14)	(40)	(5)	(11)
	118	180	7	7	24	28	13	42	6	6
	129	157	10	10	16	25	19	28	3	15
1250	(124)	(169)	(9)	(9)	(20)	(27)	(16)	(35)	(5)	(11)
	144	166	3	3	9	13	12	35	5	8
	132	142	2	7	9	19	11	27	8	4
2500	(138)	(154)	(3)	(5)	(9)	(16)	(12)	(31)	(7)	(6)
	100	148	10	8	16	9	16	22	5	10
	134	135	4	8	18	16	15	17	2	6
5000	(117)	(142)	(7)	(8)	(17)	(13)	(16)	(20)	(4)	(8)
Judgement	—	—	—	—	—	—	—	—	—	—
Specific Mutagenicity Positive Control	AF2 (711)	2AA (1178)	NaN_3 (313)	2AA (205)	AF2 (195)	2AA 20 (1397)	AF2 (491)	2AA (410)	9AA (748)	2AA (151)

Experimental Data

Con. 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+
DSMO	(158)	(153)	(12)	(12)	(27)	(29)	(24)	(21)	(9)	(7)
	142	159	10	16	32	23	20	48	5	8
20	145 (144)	152 (156)	16 (13)	14 (15)	20 (26)	16 (20)	16 (18)	39 (44)	7 (6)	6 (7)
		183		7		32		39		8
40		191 (187)		10 (9)		25 (29)		38 (39)		10 (9)
	134		13		14		24		5	
50	123 (129)		11 (12)		18 (16)		14 (19)		9 (7)	
		228		10		30		41		6
60		249 (239)		11 (11)		31 (31)		34 (38)		9 (8)
		225		13		33		31		8
80		218 (222)		9 (11)		33 (33)		49 (40)		9 (9)
	137	253	10	15	25	22	24	52	5	14
100	142 (140)	240 (247)	15 (13)	15 (15)	31 (28)	24 (23)	25 (25)	46 (49)	3 (4)	6 (10)
	139	266	13	15	26	28	20	62	8	5
200	138 (139)	279 (273)	10 (12)	11 (13)	20 (23)	26 (27)	24 (22)	54 (58)	5 (7)	2 (4)
		216		8		30		44		9
400		242 (229)		8 (8)		36 (33)		53 (49)		8 (9)
	151		9		30		26		7	
500	141 (146)		11 (10)		22 (26)		23 (25)		5 (6)	
		218		11		32		45		3
600		213 (216)		14 (13)		40 (36)		48 (47)		8 (6)
		241		11		33		52		11
800		246 (244)		13 (12)		33 (33)		51 (52)		5 (8)
	147	182	10	10	35	23	19	32	1	8
1000	146 (147)	237 (210)	6 (8)	8 (9)	21 (28)	20 (22)	20 (20)	37 (35)	7 (4)	8 (8)
	139	188	7	7	23	20	12	44	2	3
2000	136 (138)	156 (172)	6 (7)	12 (10)	21 (22)	30 (25)	11 (12)	40 (42)	2 (2)	5 (4)
	115	111	11	8	18	25	21	22	3	2
5000	129 (122)	156 (134)	9 (10)	9 (9)	24 (21)	23 (24)	21 (21)	25 (24)	3 (3)	5 (4)
Judgement	−	−	−	−	−	−	−	+	−	−
Specific Mutagenicity								280		
Positive Control	AF2 (712)	2AA (771)	NaN_3 (287)	2AA (238)	AF2 (204)	2AA 50 (1401)	AF2 (412)	2AA (389)	9AA (652)	2AA (159)

Experimental Data

Con. μg/plate	Number of Revertunts/plate	
	Base-substitution	Frame-shift
	TA100	TA98
	S9+	S9+
DSMO	(133)	(26)
	176	34
	180	54
20	(178)	(44)
	195	45
	173	39
40	(184)	(42)
	223	39
	245	43
60	(234)	(41)
	214	43
	209	43
80	(212)	(43)
	266	36
	259	53
100	(263)	(45)
	291	60
	280	45
200	(286)	(53)
	242	46
	263	59
400	(253)	(53)
	291	55
	279	63
600	(285)	(59)
	260	51
	278	68
800	(269)	(60)
	251	62
	247	50
1000	(249)	(56)
Judgement	+	+
Specific Mutagenicity	765	135
Positive Control	2AA (993)	2AA (425)