

Hexamethylene diisocyanate

[ヘキサメチレンジイソシアネート]

Experimental Data - 1

(B9317-1/3)

Chemical Name; Hexamethylene diisocyanate

Synonym ; 1,6-Diisocyanatohexane

1,6-ジイソシアナトヘキサン

Molecular Weight ; 168.20

Melting Point ; - 67 °C

Boiling Point ; 121 - 122 °C (9mmHg) [CHCD]
255 °C [Aldrich]

Flashing Point ; 140 °C [Aldrich]

Molecular Formula; C₆H₁₂N₂O₂

Chemical Structure



CAS No. ; 822-06-0

MITI No. ; (2)-2863

ML No. ; -

Specified Chemical Substances; -

Source of Substance; Tokyo Kasei Kogyo Co., Ltd.

Lot No. ; GB03

Purity ; 98 %

Vehicle ; Dehydrated DMSO

Mutagenicity in Bacterial Test ; Negative

IARC Evaluation ; not yet cited

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	(179)	(191)	(11)	(16)	(30)	(37)	(21)	(31)	(7)	(9)
	195	193	5	7	36	33	24	18	8	10
	209	186	13	22	26	33	17	31	5	13
0.0763	(202)	(190)	(9)	(15)	(31)	(33)	(21)	(25)	(7)	(12)
	187	171	16	13	34	33	21	31	16	10
	177	179	7	14	30	29	25	25	7	9
0.305	(182)	(175)	(12)	(14)	(32)	(31)	(23)	(28)	(12)	(10)
	172	186	11	15	44	34	25	34	5	11
	171	207	11	17	48	43	25	26	9	16
1.22	(172)	(197)	(11)	(16)	(46)	(39)	(25)	(30)	(7)	(14)
	201	171	16	9	21	28	17	23	2	7
	200	173	8	9	29	41	25	33	5	8
4.88	(201)	(172)	(12)	(9)	(25)	(35)	(21)	(28)	(4)	(8)
	233	206	10	14	39	31	15	28	11*	9
	188	214	15	11	25	40	43	22	13*	9
19.5	(211)	(210)	(13)	(13)	(32)	(36)	(29)	(25)	(12*)	(9)
	213*	208	0*	9	30*	28	11*	23	0*	11
	169*	190	0*	9	38*	29	14*	28	0*	10
78.1	(191*)	(199)	(0*)	(9)	(34*)	(29)	(13*)	(26)	(0*)	(11)
	0*	111*	0*	0*	0*	0*	0*	15*	0*	0*
	0*	37*	0*	0*	0*	0*	0*	9*	0*	0*
313	(0*)	(74*)	(0*)	(0*)	(0*)	(0*)	(0*)	(12*)	(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*)
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive Control	AF-2 (902)	2-AA (1309)	NaN ₃ (394)	2-AA (233)	AF-2 (210)	2-AA (1030)	AF-2 (326)	2-AA (397)	9-AA (433)	2-AA (164)

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	(141)	(139)	(10)	(13)	(31)	(36)	(17)	(29)	(7)	(9)
0.610									5 6 (6)	
1.22									7 7 (7)	
	163		8		40		25		10	
	137		10		37		16		6	
2.44	(150)		(9)		(39)		(21)		(8)	
	164		15		26		21		8	
	149		6		37		25		3	
4.88	(157)		(11)		(32)		(23)		(6)	
	184	153	8	14	21	36	29	37	10	16
	162	153	16	8	20	33	18	16	11	3
9.77	(173)	(153)	(12)	(11)	(21)	(35)	(24)	(27)	(11)	(10)
	187	148	11	7	22	47	29	28	14*	10
	178	142	10	17	30	33	21	22	11*	9
19.5	(183)	(145)	(11)	(12)	(26)	(40)	(25)	(25)	(13*)	(10)
	159*	160	8*	8	39	29	18*	20	0*	10
	187*	129	8*	10	31	34	14*	17	0*	8
39.1	(173*)	(145)	(8*)	(9)	(35)	(32)	(16*)	(19)	(0*)	(9)
	106*	172	0*	13	32*	32	0*	21		8
	122*	144	0*	11	38*	34	0*	22		11
78.1	(114*)	(158)	(0*)	(12)	(35*)	(33)	(0*)	(22)		(10)
	0*	120*	0*	10*	0*	37*	0*	22*		3*
	0*	137*	0*	8*	0*	32*	0*	15*		7*
156	(0*)	(129*)	(0*)	(9*)	(0*)	(35*)	(0*)	(19*)		(5*)
		0*		0*		0*		0*		0*
		0*		0*		0*		0*		0*
313		(0*)		(0*)		(0*)		(0*)		(0*)
		0*		0*		0*		0*		0*
		0*		0*		0*		0*		0*
625		(0*)		(0*)		(0*)		(0*)		(0*)
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive Control	AF-2 (800)	2-AA (1168)	NaN ₃ (433)	2-AA (256)	AF-2 (189)	2-AA (1021)	AF-2 (502)	2-AA (276)	9-AA (460)	2-AA (132)

Experimental Data - 3

Conc. µg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2uvrA/pKM101	
	S9-	S9+	S9-	S9+	S9-	S9+
DMSO	(294)	(355)	(305)	(426)	(69)	(119)
	268	358	338	452	78	112
	303	384	399	441	66	128
0.0763	(286)	(371)	(369)	(447)	(72)	(120)
	311	338	350	434	66	99
	290	383	317	439	76	107
0.305	(301)	(361)	(334)	(437)	(71)	(103)
	285	341	298	496	69	114
	272	396	336	439	86	155
1.22	(279)	(369)	(317)	(468)	(78)	(135)
	286	358	340	471	60	107
	286	372	335	462	82	123
4.88	(286)	(365)	(338)	(467)	(71)	(115)
	268	378	414	471	75	131
	303	378	400	492	74	117
19.5	(286)	(378)	(407)	(482)	(75)	(124)
	250	346	336*	428	71	101
	216	334	371*	488	72	109
78.1	(233)	(340)	(354*)	(458)	(72)	(105)
	0*	78*	0*	170*	0*	26*
	0*	34*	0*	0*	0*	32*
313	(0*)	(56*)	(0*)	(85*)	(0*)	(29*)
	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	2-AA	PA	2-AA	AF-2	2-AA
	(635)	(1547)	(2468)	(897)	(1166)	(742)

Experimental Data - 4

(B9317-3/3)

Conc. µg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2uvrA/pKM101	
	S9-	S9+	S9-	S9+	S9-	S9+
DMSO	(307)	(400)	(365)	(484)	(86)	(119)
	301		396			
	305		435			
2.44	(303)		(416)			
	250	406	402	492	101	99
	298	427	425	471	87	133
4.88	(274)	(417)	(414)	(482)	(94)	(116)
	284	402	477	544	77	126
	300	435	473	460	94	135
9.77	(292)	(419)	(475)	(502)	(86)	(131)
	273	417	513	538	101	128
	299	387	507	558	81	127
19.5	(286)	(402)	(510)	(548)	(91)	(128)
	246	332	472	566	86	108
	248	380	449	613	81	119
39.1	(247)	(356)	(461)	(590)	(84)	(114)
	250	322	232*	509	55*	111
	262	356	292*	541	63*	91
78.1	(256)	(339)	(262*)	(525)	(59*)	(101)
	331	314*	0*	492	0*	89*
	320	312*	0*	475	0*	93*
156	(326)	(313*)	(0*)	(484)	(0*)	(91*)
	0*	0*	0*	323*	0*	0*
	0*	0*	0*	0*	0*	0*
313	(0*)	(0*)	(0*)	(162*)	(0*)	(0*)
		0*		0*	0*	0*
		0*		0*	0*	0*
		0*		0*	0*	0*
625		(0*)		(0*)	(0*)	(0*)

Judgement — — — — —

Specific Mutagenicity

Positive Control	BLM	2-AA	PA	2-AA	AF-2	2-AA
	(630)	(2107)	(1875)	(1295)	(1519)	(958)