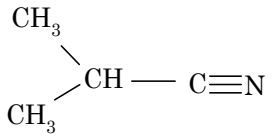
Isobutyronitrile (イソブチロニトリル)

Chemical Name ; Isobutyronitrile
Synoym ; シアン化イソプロピル
Isopropyl cyanide
2-Cyanopropane
2-Methylpropanenitrile
Molecular Weight ; 69.11
Melting Point ; -72℃[Aldrich]
Boiling Point ; 107-108℃[CHCD]
Flashing Point ; 8℃[CHCD]
Molecular Formular; C_4H_7N

Chemical Structure;



CAS No. ; 78-82-0
METI No. ; (2)-1510
MHLW No. ; −
Specified Chemical Substances; −

Source of Substance; Tokyo Kasei Kogyo Co., Ltd.
Lot No. ; FAX01
Purity ; 98%

Vehicle ; DMSO

Mutagenicity in Bacterial Test; Positive

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	(103)	(123)	(13)	(8)	(73)	(118)	(17)	(25)	(10)	(15)
	87	120	10	9	97	115	9	29	6	17
	111	139	13	10	90	117	21	23	10	15
1 .22	(99)	(130)	(12)	(10)	(94)	(116)	(15)	(26)	(8)	(16)
	107	121	10	6	75	108	15	21	7	8
	93	113	9	15	89	116	15	30	13	9
4 .88	(100)	(117)	(10)	(11)	(82)	(112)	(15)	(26)	(10)	(9)
	116	123	10	10	81	120	17	17	10	10
	83	112	9	6	84	109	11	31	6	7
19 .5	(100)	(118)	(10)	(8)	(83)	(115)	(14)	(24)	(8)	(9)
	101	112	13	6	83	122	11	23	7	15
	99	120	13	8	89	108	22	18	9	7
78 .1	(100)	(116)	(13)	(7)	(86)	(115)	(17)	(21)	(8)	(11)
	135	104	18	16	90	113	15	20	7	9
	145	134	15	10	129	157	22	16	7	20
313	(140)	(119)	(17)	(13)	(110)	(135)	(19)	(18)	(7)	(15)
	441	174	20	18	353	193	11 *	31	16 *	11
	416	157	26	14	365	241	11 *	23	26 *	9
1250	(429)	(166)	(23)	(16)	(359)	(217)	(11 *)	(27)	(21 *)	(10)
	139	449	10 *	18 *	281	1247	0 *	10 *	0 *	47 *
	176	499	9 *	9 *	301	1294	0 *	7 *	0 *	46 *
5000	(158)	(474)	(10 *)	(14 *)	(291)	(1271)	(0 *)	(9 *)	(0 *)	(47 *)
Judgement	+	+	−	+	+	+	−	−	+	+
Specific Mutagenicity	261	70.2		6.40	229	231			8.80	6.40
Positive Control	AF-2 (745)	2-AA (1280)	NaN_3 (394)	2-AA (234)	AF-2 (1218)	2-AA (938)	AF-2 (431)	2-AA (453)	9-AA (227)	2-AA (196)

* Growth inhibition was observed.

Experimental Data-2

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	(102)	(119)	(15)	(23)	(69)	(91)	(16)	(22)	(8)	(10)
39 .1	( )	( )	( )	( )	( )	( )	10 14 (12)	( )	8 10 (9)	( )
78 .1	( )	( )	( )	( )	( )	( )	14 15 (15)	( )	10 1 (6)	( )
156	116 120 (118)	129 117 (123)	23 21 (22)	24 25 (25)	79 72 (76)	81 116 (99)	18 26 (22)	15 14 (15)	7 9 (8)	11 11 (11)
313	134 119 (127)	115 127 (121)	18 11 (15)	22 23 (23)	94 105 (100)	117 108 (113)	21 24 (23)	29 23 (26)	9 10 (10)	6 11 (9)
625	246 259 (253)	141 139 (140)	16 17 (17)	21 16 (19)	185 185 (185)	114 121 (118)	28 40 (34)	31 24 (28)	22 31 (27)	13 7 (10)
1250	443 455 (449)	153 152 (153)	16 25 (21)	30 22 (26)	274 269 (272)	204 223 (214)	9 * 16 * (13 *)	44 29 (37)	6 * 14 * (10 *)	11 10 (11)
2500	310 316 (313)	225 197 (211)	7 13 (10)	14 16 (15)	229 249 (239)	740 737 (739)	0 * 0 * (0 *)	71 67 (69)	0 * 0 * (0 *)	18 17 (18)
5000	151 162 (157)	470 461 (466)	6 * 5 * (6 *)	21 * 16 * (19 *)	215 225 (220)	1143 1077 (1110)	( )	0 * 0 * (0 *)	( )	17 * 26 * (22 *)
Judgement	+	+	−	−	+	+	+	+	+	+
Specific Mutagenicity	278	69.4			186	259	28.8	18.8	30.4	2.40
Positive Control	AF-2 (704)	2-AA (1294)	NaN_3 (367)	2-AA (235)	AF-2 (1129)	2-AA (715)	AF-2 (426)	2-AA (477)	9-AA (240)	2-AA (152)

* Growth inhibition was observed.

Experimental Data-3

Conc. μg/plate	Number of Revertants/plate		
	Base-substitution	Frame-shift	
	TA1535	TA98	
	S9+	S9−	S9+
DMSO	(12)	(16)	(26)
39 .1	( )	22 13 (18)	( )
78 .1	( )	14 20 (17)	( )
156	15 13 (14)	22 17 (20)	34 34 (34)
313	16 16 (16)	17 28 (23)	23 23 (23)
625	13 15 (14)	32 31 (32)	21 26 (24)
1250	14 16 (15)	13 * 16 * (15 *)	33 29 (31)
2500	13 10 (12)	( )	77 76 (77)
5000	13 * 11 * (12 *)	( )	0 * 0 * (0 *)
Judgement	−	+	+
Specific Mutagenicity		25.6	20.4
Positive Control	2-AA (254)	AF-2 (426)	2-AA (463)

* Growth inhibition was observed.