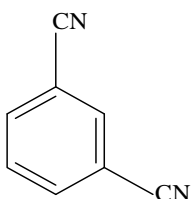


Chemical Name	: <u>1,3-Benzenedicarbonitrile</u>
Synonym	: <u>Benzene-1,3-dicarbonitrile</u> <u>1,3-Dicyanobenzene</u> <u>Isophthalonitrile</u> <u>イソフタロニトリル</u>
Molecular Weight	: 128.13
Melting Point	: 163-165°C[Aldrich]
Boiling Point	: -
Flashing Point	: -
Molecular Formula	: C ₈ H ₄ N ₂
Chemical Structure	
CAS No.	: 626-17-5
MITI No.	: (3)-1799
ML No.	: -
Specified Chemical Substances	: -
Source of Substance	: Tokyo Kasei Kogyo Co., Ltd.
Lot No.	: FHC01
Purity	: >98.0%
Vehicle	: DMSO

Conc. μ g/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2 ^{uvrA} /pKM101		TA98		TA1537	
DMSO	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
	(164)	(165)	(10)	(14)	(40)	(76)	(19)	(26)	(7)	(8)
	148	197	15	17	33	67	17	20	5	6
	151	178	11	15	38	70	20	32	5	10
1 .22	(150)	(188)	(13)	(16)	(36)	(69)	(19)	(26)	(5)	(8)
	170	188	13	11	70	84	21	28	5	7
	165	206	14	17	34	85	10	23	5	8
4 .88	(168)	(197)	(14)	(14)	(52)	(85)	(16)	(26)	(5)	(8)
	163	178	15	18	43	75	24	25	5	10
	167	173	10	10	47	77	22	17	8	3
19 .5	(165)	(176)	(13)	(14)	(45)	(76)	(23)	(21)	(7)	(7)
	170	194	8	13	29	77	14	15	6	10
	179	165	14	9	49	74	11	26	5	9
78 .1	(175)	(180)	(11)	(11)	(39)	(76)	(13)	(21)	(6)	(10)
	169	171	6	8	40	64	15	22	2	10
	171	171	10	18	39	83	18	25	5	9
313	(170)	(171)	(8)	(13)	(40)	(74)	(17)	(24)	(4)	(10)
	137	158	10	13	53	72	16	36	6	10
	156	165	5	9	41	64	23	24	6	8
1250	(147)	(162)	(8)	(11)	(47)	(68)	(20)	(30)	(6)	(9)
	116	94	9	8	33	40	14	28	3	5
	116	121	7	10	39	49	15	17	5	9
5000	(116)	(108)	(8)	(9)	(36)	(45)	(15)	(23)	(4)	(7)
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive Control	AF-2 (560)	2-AA (1080)	NaN ₃ (394)	2-AA (265)	AF-2 (670)	2-AA (739)	AF-2 (483)	2-AA (421)	9-AA (564)	2-AA (194)

Mutagenicity in Bacterial Test ; Negative

IARC Evaluation ; not yet cited

Experimental Data-2

(B9803-2/2)

Conc. μ g/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA/pKM101		TA98		TA1537	
DMSO	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
		(147)	(174)	(8)	(9)	(35)	(51)	(15)	(23)	(6)
313	137	155	8	11	38	52	10	20	3	8
	(144)	(164)	(9)	(9)	(36)	(50)	(15)	(23)	(5)	(7)
625	148	152	6	17	45	44	9	17	5	7
	(160)	(166)	(7)	(15)	(42)	(54)	(13)	(21)	(6)	(7)
1250	137	163	8	7	54	60	14	20	3	8
	(148)	(164)	(11)	(7)	(48)	(57)	(14)	(20)	(4)	(9)
2500	134	150	6	9	24	54	15	17	3	10
	(137)	(152)	(7)	(9)	(31)	(43)	(15)	(15)	(6)	(10)
5000	99	120	7	13	24	51	9	14	7	3
	(111)	(118)	(8)	(11)	(25)	(43)	(12)	(13)	(7)	(5)
Judgement	—	—	—	—	—	—	—	—	—	—
Specific Mutagenicity										
Positive Control	AF-2 (540)	2-AA (1026)	NaN ₃ (352)	2-AA (270)	AF-2 (599)	2-AA (553)	AF-2 (517)	2-AA (446)	9-AA (401)	2-AA (183)