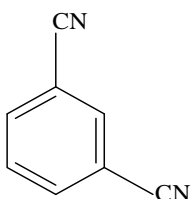


Chemical Name	: <u>1,3-Benzenedicarbonitrile</u>
Synonym	: <u>Benzene-1,3-dicarbonitrile</u> <u>1,3-Dicyanobenzene</u> <u>Isophthalonitrile</u> <u>イソフタロニトリル</u>
Molecular Weight	: 128.13
Melting Point	: 163-165°C[Aldrich]
Boiling Point	: -
Flashing Point	: -
Molecular Formula	: C ₈ H ₄ N ₂
Chemical Structure	
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)
1 .22	148 151 (150)	197 178 (188)	15 11 (13)	17 15 (16)	33 38 (36)	67 70 (69)	17 20 (19)	20 32 (26)	5 5 (5)	6 10 (8)
4 .88	170 165 (168)	188 206 (197)	13 14 (14)	11 17 (14)	70 34 (52)	84 85 (85)	21 10 (16)	28 23 (26)	5 5 (5)	7 8 (8)
19 .5	163 167 (165)	178 173 (176)	15 10 (13)	18 10 (14)	43 47 (45)	75 77 (76)	24 22 (23)	25 17 (21)	5 8 (7)	10 3 (7)
78 .1	170 179 (175)	194 165 (180)	8 14 (11)	13 9 (11)	29 49 (39)	77 74 (76)	14 11 (13)	15 26 (21)	6 5 (6)	10 9 (10)
313	169 171 (170)	171 171 (171)	6 10 (8)	8 18 (13)	40 39 (40)	64 83 (74)	15 18 (17)	22 25 (24)	2 5 (4)	10 9 (10)
1250	137 156 (147)	158 165 (162)	10 5 (8)	13 9 (11)	53 41 (47)	72 64 (68)	16 23 (20)	36 24 (30)	6 6 (6)	10 8 (9)
5000	116 116 (116)	94 121 (108)	9 7 (8)	8 10 (9)	33 39 (36)	40 49 (45)	14 15 (15)	28 17 (23)	3 5 (4)	5 9 (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)	(8)
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)