

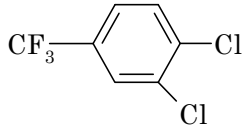
1,2-Dichloro-4-(trifluoromethyl)benzene

(1,2-ジクロロ-4-(トリフルオロメチル)ベンゼン)

Chemical Name ; 1,2-Dichloro-4-(trifluoromethyl)benzene
 Synonym ; 3,4-Dichlorobenzotrifluoride
3,4-Dichloro- α, α, α -trifluorotoluene

Molecular Weight ; 215.00
 Melting Point ; -13 - -12 °C[Aldrich]
 Boiling Point ; 173-174 °C[CHCD]
 Flashing Point ; 65.6°C[Aldrich]
 Molecular Formular; C₇H₃Cl₂F₃

Chemical Structure:



CAS No. ; 328-84-7
 METI No. ; (3)-3553
 MHLW No. ; 4-(15)-58
 Specified Chemical Substances; -

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

Lot No. ; GA01
 Purity ; >95%

Vehicle ; DMSO

Mutagenicity in Bacterial Test; Negative

IARC Evaluation ; not yet cited

Conc. μ g/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2 <i>uvrA</i> /pKM101		TA98		TA1537	
DMSO	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
		(115)	(122)	(13)	(8)	(55)	(86)	(15)	(25)	(6)
	122	156	17	10	56	98	10	24	3	13
1 .22	(126)	(138)	(12)	(9)	(62)	(96)	(16)	(23)	(3)	(11)
	105	135	10	2	51	136	17	29	11	14
4 .88	(117)	(141)	(11)	(5)	(57)	(125)	(16)	(27)	(10)	(9)
	94	127	9	11	67	105	20	25	9	6
19 .5	(105)	(133)	(11)	(10)	(62)	(107)	(18)	(24)	(8)	(6)
	61 *	129	5 *	2	39 *	85	9 *	17	8 *	16
78 .1	(64 *)	(117)	(6 *)	(5)	(30 *)	(85)	(9 *)	(23)	(6 *)	(12)
	67 *	104	7 *	8	20 *	85	8 *	29	3 *	8
	69 *	89 *	2 *	3 *	29 *	41 *	10 *	8 *	7 *	7 *
313	(59 *)	(94 *)	(2 *)	(4 *)	(31 *)	(42 *)	(9 *)	(11 *)	(7 *)	(7 *)
	48 *	98 *	2 *	5 *	33 *	43 *	8 *	13 *	7 *	7 *
	0 *	97 *	0 *	7 *	0 *	45 *	0 *	13 *	0 *	3 *
1250	(0 *)	(92 *)	(0 *)	(7 *)	(0 *)	(38 *)	(0 *)	(12 *)	(0 *)	(3 *)
	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 (774)	2-AA (1321)	NaN ₃ (460)	2-AA (295)	AF-2 (1304)	2-AA (1088)	AF-2 (476)	2-AA (487)	9-AA (439)	2-AA (267)

* Growth inhibition was observed.

Experimental Data-2

(B9907-2/3)

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+
	(128)	(128)	(11)	(8)	(61)	(94)	(17)	(20)	(11)	(15)
2 .44	129 114 (122)	()	8 9 (9)	()	71 71 (71)	()	10 7 (9)	()	16 9 (13)	()
4 .88	115 106 (111)	()	10 6 (8)	()	91 59 (75)	()	13 15 (14)	()	10 20 (15)	()
9 .77	123 123 (123)	131 123 (127)	8 13 (11)	9 2 (6)	71 57 (64)	90 113 (102)	8 15 (12)	30 31 (31)	9 13 (11)	22 18 (20)
19 .5	108 116 (112)	141 119 (130)	10 8 (9)	8 13 (11)	45 68 (57)	107 92 (100)	17 23 (20)	22 25 (24)	11 14 (13)	14 17 (16)
39 .1	96 * 82 * (89 *)	115 128 (122)	5 * 5 * (5 *)	3 13 (8)	62 * 59 * (61 *)	120 115 (118)	16 * 17 * (17 *)	28 20 (24)	2 * 8 * (5 *)	16 16 (16)
78 .1	71 * 94 * (83 *)	116 115 (116)	2 * 11 * (7 *)	9 2 (6)	31 * 28 * (30 *)	86 91 (89)	7 * 15 * (11 *)	23 21 (22)	1 * 9 * (5 *)	8 11 (10)
156		96 * 72 * (84 *)		3 * 1 * (2 *)		54 * 79 * (67 *)		10 * 14 * (12 *)		2 * 6 * (4 *)
313		121 * 87 * (104 *)		6 * 3 * (5 *)		52 * 40 * (46 *)		15 * 28 * (22 *)		7 * 7 * (7 *)
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive Control	AF-2 (744)	2-AA (1535)	NaN ₃ (435)	2-AA (259)	AF-2 (874)	2-AA (956)	AF-2 (470)	2-AA (473)	9-AA (435)	2-AA (249)

* Growth inhibition was observed.

Experimental Data-3

(B9907-3/3)

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-
	(112)	(9)	(73)	(20)	(8)
	115	11	60	17	5
2 .44	101	11	72	13	11
	(108)	(11)	(66)	(15)	(8)
	115	8	67	18	9
4 .88	126	10	76	18	3
	(121)	(9)	(72)	(18)	(6)
	109	9	77	7	6
9 .77	115	15	75	18	5
	(112)	(12)	(76)	(13)	(6)
	93	6	64	13	3
19 .5	111	13	68	15	6
	(102)	(10)	(66)	(14)	(5)
	111 *	10 *	72 *	18 *	7 *
39 .1	102 *	9 *	70 *	11 *	13 *
	(107 *)	(10 *)	(71 *)	(15 *)	(10 *)
	Judgement	-	-	-	-
Specific Mutagenicity					
Positive Control	AF-2 (641)	NaN ₃ (416)	AF-2 (1005)	AF-2 (496)	9-AA (316)

* Growth inhibition was observed.