

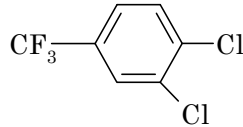
## 1,2-Dichloro-4-(trifluoromethyl)benzene

(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- $\alpha, \alpha, \alpha$ -trifluorotoluene

Molecular Weight ; 215.00  
 Melting Point ; -13 - -12 °C[Aldrich]  
 Boiling Point ; 173-174 °C[CHCD]  
 Flashing Point ; 65.6°C[Aldrich]  
 Molecular Formula; C<sub>7</sub>H<sub>3</sub>Cl<sub>2</sub>F<sub>3</sub>

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

Conc. $\mu$ 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 <sub>3</sub> ( 460 )	2-AA ( 295 )	AF-2 ( 1304 )	2-AA ( 1088 )	AF-2 ( 476 )	2-AA ( 487 )	9-AA ( 439 )	2-AA ( 267 )

Mutagenicity in Bacterial Test; Negative

IARC Evaluation ; not yet cited

\* 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 <sub>uvrA</sub> /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		8		71		10		16	
	114		9		71		7		9	
	( 122 )	( )	( 9 )	( )	( 71 )	( )	( 9 )	( )	( 13 )	( )
4 .88	115		10		91		13		10	
	106		6		59		15		20	
	( 111 )	( )	( 8 )	( )	( 75 )	( )	( 14 )	( )	( 15 )	( )
9 .77	123	131	8	9	71	90	8	30	9	22
	123	123	13	2	57	113	15	31	13	18
	( 123 )	( 127 )	( 11 )	( 6 )	( 64 )	( 102 )	( 12 )	( 31 )	( 11 )	( 20 )
19 .5	108	141	10	8	45	107	17	22	11	14
	116	119	8	13	68	92	23	25	14	17
	( 112 )	( 130 )	( 9 )	( 11 )	( 57 )	( 100 )	( 20 )	( 24 )	( 13 )	( 16 )
39 .1	96 *	115	5 *	3	62 *	120	16 *	28	2 *	16
	82 *	128	5 *	13	59 *	115	17 *	20	8 *	16
	( 89 *)	( 122 )	( 5 *)	( 8 )	( 61 *)	( 118 )	( 17 *)	( 24 )	( 5 *)	( 16 )
78 .1	71 *	116	2 *	9	31 *	86	7 *	23	1 *	8
	94 *	115	11 *	2	28 *	91	15 *	21	9 *	11
	( 83 *)	( 116 )	( 7 *)	( 6 )	( 30 *)	( 89 )	( 11 *)	( 22 )	( 5 *)	( 10 )
156		96 *		3 *		54 *		10 *		2 *
		72 *		1 *		79 *		14 *		6 *
		( 84 *)		( 2 *)		( 67 *)		( 12 *)		( 4 *)
313		121 *		6 *		52 *		15 *		7 *
		87 *		3 *		40 *		28 *		7 *
		( 104 *)		( 5 *)		( 46 *)		( 22 *)		( 7 *)
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive Control	AF-2 ( 744 )	2-AA ( 1535 )	NaN <sub>3</sub> ( 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 <sub>uvrA</sub> /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 <sub>3</sub> ( 416 )	AF-2 ( 1005 )	AF-2 ( 496 )	9-AA ( 316 )

\* Growth inhibition was observed.