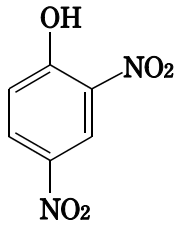
Chemical Name;2,4-Dinitrophenol
Synonym ;α-Dinitrophenol
α-ジニトロフェノール

Molecular Weight ; 184.11
Melting Point ; 113 ℃ [CHCD]
106 - 108 ℃ [Aldrich,CHCD]
112 - 114 ℃ [Merck]
Boiling Point ; — ℃
Flashing Point ; — ℃
Molecular Formula; $C_6H_4N_2O_5$

Chemical Structure



CAS No. ; 51-28-5
MITI No. ; (3)-797
ML No. ; —
Specified Chemical Substances; —

Source of Substance; Tokyo Kasei Kogyo Co.,Ltd.
Lot No. ; FHA01
Purity ; 98 - 99 %

Vehicle ; DMSO

Mutagenicity in Bacterial Test ; **Negative**

IARC Evaluation ; not yet cited

Conc. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2*uvrA*		TA98		TA1537	
	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+
DMSO	(181)	(191)	(7)	(13)	(30)	(38)	(18)	(28)	(7)	(11)
	179	177	5	18	32	39	25	36	7	9
	185	178	14	18	23	32	23	39	8	10
0.0763	(182)	(178)	(10)	(18)	(28)	(36)	(24)	(38)	(8)	(10)
	164	192	9	14	22	38	34	33	6	10
	188	171	10	13	31	38	17	25	6	9
0.305	(176)	(182)	(10)	(14)	(27)	(38)	(26)	(29)	(6)	(10)
	205	183	5	9	28	40	8	28	8	14
	178	185	10	11	24	40	24	29	7	6
1.22	(192)	(184)	(8)	(10)	(26)	(40)	(16)	(29)	(8)	(10)
	198	214	13	10	16	37	22	37	7	11
	183	184	10	15	38	38	15	39	8	11
4.88	(191)	(199)	(12)	(13)	(27)	(38)	(19)	(38)	(8)	(11)
	166	204	11	17	28	30	20	37	8	11
	222	188	9	11	34	46	15	28	5	14
19.5	(194)	(196)	(10)	(14)	(31)	(38)	(18)	(33)	(7)	(13)
	176	186	17	10	38	41	22	28	7	8
	184	167	15	14	31	30	22	28	14	10
78.1	(180)	(177)	(16)	(12)	(35)	(36)	(22)	(28)	(11)	(9)
	178	172	5	10	29	22	25	23	7	7
	177	143	8	10	20	31	34	26	7	8
313	(178)	(158)	(7)	(10)	(25)	(27)	(30)	(25)	(7)	(8)
	71*	0*	1*	2*	11*	18*	17*	0*	1*	1*
	61*	0*	2*	0*	14*	25*	15*	0*	1*	1*
1250	(66*)	(0*)	(2*)	(1*)	(13*)	(22*)	(16*)	(0*)	(1*)	(1*)
	0*	0*	0*	0*	0*	3*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	5*	0*	0*	0*	0*
5000	(0*)	(0*)	(0*)	(0*)	(0*)	(4*)	(0*)	(0*)	(0*)	(0*)
Judgement	—	—	—	—	—	—	—	—	—	—
Specific Mutagenicity										
Positive Control	AF-2 (907)	2-AA (1362)	NaN_3 (396)	2-AA (237)	AF-2 (206)	2-AA (1027)	AF-2 (329)	2-AA (397)	9-AA (438)	2-AA (164)

Conc. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2*uvrA*		TA98		TA1537	
	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+
DMSO	(154)	(164)	(10)	(11)	(31)	(41)	(17)	(26)	(7)	(10)
	165	184	13	14	24	23	14	25	5	9
	173	160	8	11	28	36	10	30	9	9
39.1	(169)	(172)	(11)	(13)	(26)	(30)	(12)	(28)	(7)	(9)
	190	152	6	9	40	37	30	30	9	9
	188	167	5	14	34	41	14	21	8	13
78.1	(189)	(160)	(6)	(12)	(37)	(39)	(22)	(26)	(9)	(11)
	152	155	8	15	30	38	18	33	13	5
	164	142	13	10	31	41	14	40	2	5
156	(158)	(149)	(11)	(13)	(31)	(40)	(16)	(37)	(8)	(5)
	155	165	13	8	36	26	20	26	7	8
	162	137	11	10	26	29	25	28	18	8
313	(159)	(151)	(12)	(9)	(31)	(28)	(23)	(27)	(13)	(8)
	151	120	5	3	21	33	13	11	1	5
	152	149	1	6	25	23	22	23	6	8
625	(152)	(135)	(3)	(5)	(23)	(28)	(18)	(17)	(4)	(7)
	59*	13*	0*	0*	10*	15*	0*	0*	0*	0*
	46*	11*	5*	0*	29*	23*	1*	0*	0*	0*
1250	(53*)	(12*)	(3*)	(0*)	(20*)	(19*)	(1*)	(0*)	(0*)	(0*)
	0*	0*	0*	0*	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*	0*	0*	0*	0*
2500	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
Judgement	−	−	−	−	−	−	−	−	−	−
Specific Mutagenicity										
Positive Control	AF-2 (779)	2-AA (1133)	NaN_3 (401)	2-AA (247)	AF-2 (185)	2-AA (1005)	AF-2 (491)	2-AA (274)	9-AA (443)	2-AA (131)

Experimental Data - 3

Conc. μg/plate	Number of Revertants/plate Base-substitution TA1535 S9−	S9+
DMSO	(11)	(13)
	21	11
	11	15
78.1	(16)	(13)
	20	10
	8	13
156	(14)	(12)
	11	10
	11	13
313	(11)	(12)
	11	11
	9	7
625	(10)	(9)
	6*	0*
	6*	0*
1250	(6*)	(0*)
	0*	0*
	0*	0*
2500	(0*)	(0*)
	0*	0*
	0*	0*
5000	(0*)	(0*)
Judgement	−	−
Specific Mutagenicity		
Positive Control	NaN_3 (410)	2-AA (248)

Experimental Data - 4

(B9312-3/4)

Conc. μg/plate	Number of Revertants/plate Base-substitution TA102 S9−	S9+	TA104 S9−	S9+	WP2*uvrA*/pKM101 S9−	S9+
DMSO	(297)	(363)	(386)	(509)	(89)	(105)
	306	383	400	483	84	109
	293	400	383	480	97	123
0.0763	(300)	(392)	(392)	(482)	(91)	(116)
	313	422	407	503	77	104
	271	382	439	465	71	120
0.305	(292)	(402)	(423)	(484)	(74)	(112)
	286	376	401	507	81	100
	265	406	378	452	72	114
1.22	(276)	(391)	(390)	(480)	(77)	(107)
	249	374	372	422	74	120
	274	366	416	478	60	136
4.88	(262)	(370)	(394)	(450)	(67)	(128)
	245	358	349	498	78	99
	236	322	385	457	81	102
19.5	(241)	(340)	(367)	(478)	(80)	(101)
	115	201	376	482	60	100
	100	204	340	436	67	92
78.1	(108)	(203)	(358)	(459)	(64)	(96)
	1*	2*	341	358	23*	62*
	6*	13*	310	317	34*	66*
313	(4*)	(8*)	(326)	(338)	(29*)	(64*)
	1*	1*	72*	49*	0*	10*
	2*	7*	60*	20*	0*	7*
1250	(2*)	(4*)	(66*)	(35*)	(0*)	(9*)
	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*
5000	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
Judgement	−	−	−	−	−	−
Specific Mutagenicity						
Positive Control	BLM (630)	2-AA (563)	PA (1682)	2-AA (1220)	AF-2 (1515)	2-AA (962)

Experimental Data - 5

Conc. μg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2*uvrA*/pKM101	
	S9−	S9+	S9−	S9+	S9−	S9+
DMSO	(226)	(319)	(337)	(408)	(44)	(67)
	240	287			52	55
	230	301			46	66
4.88	(235)	(294)			(49)	(61)
	232	316			49	79
	222	294			37	69
9.77	(227)	(305)			(43)	(74)
	191	306	338	417	54	63
	214	276	344	438	46	68
19.5	(203)	(291)	(341)	(428)	(50)	(66)
	134	268	335	430	34	56
	160	234	320	416	43	56
39.1	(147)	(251)	(328)	(423)	(39)	(56)
	100	160	368	383	34	54
	130	155	343	427	38	60
78.1	(115)	(158)	(356)	(405)	(36)	(57)
	40	75	341	361	39*	53
	36	85	356	396	48*	62
156	(38)	(80)	(349)	(379)	(44*)	(58)
	14*	22*	292	353	33*	46*
	10*	8*	298	358	25*	44*
313	(12*)	(15*)	(295)	(356)	(29*)	(45*)
	3*	3*	280*	306*	15*	34*
	6*	3*	221*	305*	9*	24*
625	(5*)	(3*)	(251*)	(306*)	(12*)	(29*)
			69*	57*		
			56*	39*		
1250			(63*)	(48*)		
			6*	7*		
			5*	24*		
2500			(6*)	(16*)		
Judgement	−	−	−	−	−	−
Specific Mutagenicity						
Positive Control	BLM (708)	2-AA (1198)	PA (948)	2-AA (898)	AF-2 (723)	2-AA (542)