

Diketene (ジケテン)

Chemical Name:	Diketene
Synonym	4-Methylene-2-oxetanone Acetyl ketene Oxetanone, 4-methylene-
Molecular weight:	84.08
Melting point:	-6.5°C
Boiling point:	127.4°C, 69~70°C (100mmHg)
Flashing point:	34°C
Chemical Structure	$\begin{array}{c} \text{CH}_2 = \text{C} - \text{CH}_2 \\ \quad \\ \text{O} - \text{C} = \text{O} \end{array}$
CAS No :	674-82-8
MITI No:	(5)-13
Source of Substance:	Wako Pure Chem. Ind., Ltd.
Lot.No.:	SAN5723
Purity:	99 %
Vehicle:	Acetone

Mutagenicity
in Bacterial Test: Negative

IARC Evaluation: not yet cited

Con. μg/ plate	Experimental Data									
	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA		TA98		TA1537	
	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
Acetone	(148)	(167)	(8)	(11)	(19)	(22)	(21)	(23)	(7)	(8)
	132	176	10	10	24	21	25	23	3	10
9.77	(134)	(175)	(11)	(9)	(22)	(22)	(23)	(20)	(5)	(8)
	173	187	9	12	22	25	14	20	3	9
19.5	(161)	(180)	(10)	(12)	(19)	(23)	(14)	(21)	(4)	(9)
	151	173	12	8	18	25	17	20	5	8
39.1	(163)	(181)	(8)	(8)	(20)	(24)	(19)	(21)	(6)	(8)
	170	177	9	5	18	25	22	24	8	6
78.1	(153)	(172)	(8)	(6)	(22)	(24)	(23)	(24)	(7)	(6)
	136	166	7	7	25	22	24	24	6	5
156	(143)	(183)	(4)	(8)	(25)	(22)	(33)	(28)	(7)	(7)
	151	185	2	10	25	24	39	27	7	8
	135	180	5	6	24	20	27	28	6	5
313	(59*)	(159)	(0*)	(11)	(17*)	(21)	(3*)	(20)	(0*)	(8)
	60*	148	0*	10	17*	18	5*	17	0*	8
	57*	169	0*	12	16*	24	0*	23	0*	8
625	(0*)	(175)	(0*)	(10)	(17*)	(27)	(0*)	(36)	(0*)	(8)
	0*	62*	0*	3*	0*	18*	0*	5*	0*	3*
	0*	68*	0*	5*	0*	18*	0*	8*	0*	7*
1250	(0*)	(65*)	(0*)	(4*)	(0*)	(18*)	(0*)	(7*)	(0*)	(5*)
	0*	69*	0*	0*	0*	0*	0*	0*	0*	0*
	0*	65*	0*	0*	0*	0*	0*	0*	0*	0*
2500	(0*)	(67*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
5000	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
Judgement	—									
Specific Mutagenicity	—									
Positive Control	AF2	2AA	NaN ₃	2AA	AF2	2AA 20	AF2	2AA	9AA	2AA
Control	(735)	(943)	(243)	(243)	(219)	(1011)	(364)	(425)	(546)	(197)

Experimental Data

Con. μ g/ plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA		TA98		TA1537	
	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
Acetone	(190)	(184)	(11)	(10)	(24)	(26)	(21)	(22)	(8)	(14)
	172		16		28		15		7	
	184		12		29		16		5	
9.77	(178)		(14)		(29)		(16)		(6)	
	170		7		22		17		8	
	164		15		30		17		7	
19.5	(167)		(11)		(26)		(17)		(8)	
	158	185	16	17	23	27	20	27	8	14
	192	194	8	13	29	23	20	25	3	13
39.1	(175)	(190)	(12)	(15)	(26)	(25)	(20)	(26)	(6)	(14)
	175	193	10	7	23	27	17	24	12	16
	168	193	12	13	30	34	20	21	8	15
78.1	(172)	(193)	(11)	(10)	(27)	(31)	(19)	(23)	(10)	(16)
	163	193	10	15	24	31	24	23	10	16
	150	206	10	9	18	30	22	28	2	13
156	(157)	(200)	(10)	(12)	(21)	(31)	(23)	(26)	(6)	(15)
	108*	170	0*	8	22*	28	6*	24	0*	14
	109*	175	0*	12	22*	30	9*	22	0*	15
313	(109*)	(173)	(0*)	(10)	(22*)	(29)	(8*)	(23)	(0*)	(15)
	0*	160	0*	7	0*	29	0*	25	0*	9
	0*	157	0*	7	0*	25	0*	28	0*	8
625	(0*)	(159)	(0*)	(7)	(0*)	(27)	(0*)	(27)	(0*)	(9)
		125*		6*		22*		8*		5*
		131*		6*		16*		13*		5*
1250		(128*)		(6*)		(19*)		(11*)		(5*)
		0*		0*		0*		0*		0*
		0*		0*		0*		0*		0*
2500		(0*)		(0*)		(0*)		(0*)		(0*)
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive	AF2	2AA	NaN ₃	2AA	AF2	2AA 20	AF2	2AA	9AA	2AA
Control	(727)	(683)	(366)	(196)	(223)	(1177)	(397)	(371)	(598)	(172)

Con. μg/ plate	Experimental Data					
	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2uvrA/pKM101	
	S9-	S9+	S9-	S9+	S9-	S9+
Acetone	(203)	(251)	(222)	(227)	(95)	(124)
	223		194		81	
	208		220		68	
9.77	(216)		(207)		(75)	
	191		194		87	
	190		212		88	
19.5	(191)		(203)		(88)	
	177	244	212	206	103	131
	184	245	235	210	83	123
39.1	(181)	(245)	(224)	(208)	(93)	(127)
	185	231	243	187	86	114
	181	266	232	242	99	92
78.1	(183)	(249)	(238)	(215)	(93)	(103)
	135	224	245	236	106	106
	141	253	247	185	110	120
156	(138)	(239)	(246)	(211)	(108)	(113)
	66*	190	201*	217	42*	120
	28*	214	154*	235	59*	126
313	(47*)	(202)	(178*)	(226)	(51*)	(123)
	0*	147*	0*	268*	0*	135
	0*	116*	0*	227*	0*	123*
625	(0*)	(132*)	(0*)	(248*)	(0*)	(129*)
		0*		13*		29*
		0*		15*		15*
1250		(0*)		(14*)		(22*)
		0*		0*		0*
		0*		0*		0*
2500		(0*)		(0*)		(0*)
Judgement	-	-	-	-	-	-
Specific Mutagenicity						
Positive	BLM	2AA	PA	2AA	AF2	2AA
Control	(475)	(983)	(1310)	(1127)	(569)	(494)