

Chemical Name	: <u>Methyl acetoacetate</u>
Synonym	: <u>Methyl 3-oxobutanoate</u> <u>3-Oxobutanoic acid methyl ester</u> <u>3-オキソブタン酸メチル</u>
Molecular Weight	: 116.12
Melting Point	: -80°C [Aldrich]
Boiling Point	: 169-170°C [Aldrich]
Flashing Point	: 82°C [Merch]
Molecular Formula	: C ₅ H ₈ O ₃
Chemical Structure	<chem>CC(=O)CH2COOCH3</chem>
CAS No.	: 105-45-3
MITI No.	: (2)-1474, (2)-1475
ML No.	: -
Specified Chemical Substances	: -
Source of Substance	: Tokyo Kasei Kogyo Co., Ltd.
Lot No.	: GD01
Purity	: 99.0%
Vehicle	: Distilled H ₂ O

Conc. μ g/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA/pKM101		TA98		TA1537	
H ₂ O	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
		(133)	(143)	(8)	(11)	(44)	(75)	(15)	(23)	(5)
1 .22	128	149	9	7	44	62	20	24	3	10
	(129)	(149)	(10)	(9)	(46)	(74)	(17)	(20)	(3)	(10)
4 .88	124	145	6	16	44	78	10	30	5	6
	(135)	(145)	(9)	(15)	(53)	(75)	(13)	(28)	(6)	(6)
19 .5	138	163	14	20	45	74	16	20	6	6
	(125)	(145)	(11)	(18)	(59)	(71)	(17)	(23)	(5)	(8)
78 .1	131	143	7	9	69	97	16	28	2	6
	(133)	(144)	(7)	(10)	(69)	(84)	(16)	(26)	(2)	(8)
313	138	146	6	8	111	79	31	29	7	13
	(142)	(148)	(7)	(8)	(108)	(88)	(28)	(27)	(4)	(11)
1250	131	145	8	17	146	144	21	15	6	10
	(133)	(143)	(9)	(16)	(150)	(143)	(22)	(20)	(6)	(11)
5000	124	162	6	11	151	288	20	21	7	18
	(128)	(160)	(10)	(13)	(125)	(271)	(18)	(23)	(5)	(14)
Judgement	-	-	-	-	+	+	-	-	-	-
Specific Mutagenicity					204	39.2				
Positive Control	AF-2 (806)	2-AA (1583)	NaN ₃ (402)	2-AA (363)	AF-2 (1979)	2-AA (1102)	AF-2 (473)	2-AA (462)	9-AA (829)	2-AA (249)

Mutagenicity in Bacterial Test ; Positive

IARC Evaluation ; not yet cited

Experimental Data-2

(B9702-2/2)

Conc. μ g/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2 _{uvrA} /pKM101		TA98		TA1537	
H ₂ O	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
	(141)	(157)	(7)	(11)	(33)	(58)	(17)	(28)	(6)	(8)
39 .1					54 39 (47)	61 71 (66)				
78 .1					63 70 (67)	66 78 (72)				
156					74 77 (76)	63 55 (59)				
313	163 177 (170)	163 183 (173)	11 8 (10)	10 10 (10)	66 87 (77)	76 89 (83)	15 15 (15)	26 30 (28)	5 6 (6)	8 5 (7)
625	166 173 (170)	166 171 (169)	5 5 (5)	11 8 (10)	130 111 (121)	72 86 (79)	18 23 (21)	32 25 (29)	5 8 (7)	10 10 (10)
1250	130 160 (145)	173 187 (180)	8 8 (8)	9 5 (7)	109 120 (115)	105 145 (125)	17 17 (17)	24 31 (28)	3 3 (3)	10 6 (8)
2500	137 159 (148)	174 144 (159)	9 9 (9)	11 16 (14)	116 130 (123)	158 198 (178)	17 21 (19)	23 18 (21)	9 6 (8)	3 10 (7)
5000	156 142 (149)	153 179 (166)	7 7 (7)	14 11 (13)	135 130 (133)	246 235 (241)	20 23 (22)	20 15 (18)	6 5 (6)	10 5 (8)
Judgement	-	-	-	-	+	+	-	-	-	-
Specific Mutagenicity					435	53.6				
Positive Control	AF-2 (659)	2-AA (1219)	NaN ₃ (473)	2-AA (361)	AF-2 (732)	2-AA (876)	AF-2 (518)	2-AA (442)	9-AA (669)	2-AA (201)