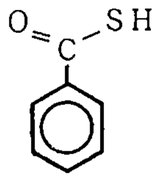
Thiobenzoic acid (チオ安息香酸)

Chemical Name: Thiobenzoic acid
Synonym Benzenecarbothioic acid
Molecular weight: 138.18
Melting point: 15-18℃
Boiling point: 122℃ (30mmHg), 95~97℃
Flashing point: > 110℃
Chemical Structure



CAS NO : 98-91-9
MITI NO: (3)-1396
Source of Substance:Tokyo Kasei Kogyo Co.Ltd
Lot.No.: AV01
Purity: ≧ 95 %
Vehicle: Acetone

Mutagenicity
in Bacterial Test : Negative

IARC Evaluation :not yet citied

Experimental Data

| Con. μg/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 | ( 162 ) | ( 177 ) | ( 10 ) | ( 10 ) | ( 42 ) | ( 41 ) | ( 21 ) | ( 22 ) | ( 5 ) | ( 12 ) |
| | 168 | 194 | 9 | 12 | 33 | 34 | 17 | 27 | 10 | 14 |
| | 164 | 173 | 7 | 12 | 37 | 26 | 16 | 24 | 5 | 7 |
| 9.77 | ( 166 ) | ( 184 ) | ( 8 ) | ( 12 ) | ( 35 ) | ( 30 ) | ( 17 ) | ( 26 ) | ( 8 ) | ( 11 ) |
| | 144 | 185 | 13 | 9 | 41 | 37 | 21 | 27 | 5 | 10 |
| | 169 | 182 | 5 | 14 | 48 | 34 | 22 | 23 | 9 | 9 |
| 19.5 | ( 157 ) | ( 184 ) | ( 9 ) | ( 12 ) | ( 45 ) | ( 36 ) | ( 22 ) | ( 25 ) | ( 7 ) | ( 10 ) |
| | 140 | 182 | 4 | 9 | 40 | 45 | 22 | 24 | 6 | 18 |
| | 161 | 191 | 8 | 11 | 29 | 36 | 16 | 33 | 7 | 10 |
| 39.1 | ( 151 ) | ( 187 ) | ( 6 ) | ( 10 ) | ( 35 ) | ( 41 ) | ( 19 ) | ( 29 ) | ( 7 ) | ( 14 ) |
| | 111 | 163 | 10 | 8 | 40 | 51 | 20 | 21 | 5 | 11 |
| | 105 | 177 | 7 | 11 | 37 | 46 | 14 | 31 | 5 | 12 |
| 78.1 | ( 108 ) | ( 170 ) | ( 9 ) | ( 10 ) | ( 39 ) | ( 49 ) | ( 17 ) | ( 26 ) | ( 5 ) | ( 12 ) |
| | 92* | 206 | 8 | 17 | 40 | 42 | 34 | 30 | 9 | 11 |
| | 76* | 155 | 7* | 11 | 37 | 44 | 16 | 28 | 7 | 10 |
| 156 | ( 84*) | ( 181 ) | ( 8*) | ( 14 ) | ( 39 ) | ( 43 ) | ( 25 ) | ( 29 ) | ( 8 ) | ( 11 ) |
| | 0* | 185 | 11* | 11 | 39 | 42 | 23 | 22 | 5 | 18 |
| | 0* | 176 | 4* | 8 | 35 | 29 | 23 | 23 | 5 | 12 |
| 313 | ( 0*) | ( 181 ) | ( 8*) | ( 10 ) | ( 37 ) | ( 36 ) | ( 23 ) | ( 23 ) | ( 5 ) | ( 15 ) |
| | 0* | 173 | 0* | 3 | 36 | 41 | 22 | 23 | 6 | 6 |
| | 0* | 185 | 0* | 9 | 33 | 40 | 5* | 22 | 9 | 5 |
| 625 | ( 0*) | ( 179 ) | ( 0*) | ( 6 ) | ( 35 ) | ( 41 ) | ( 14*) | ( 23 ) | ( 8 ) | ( 6 ) |
| | 0* | 150 | 0* | 12 | 37 | 35 | 0* | 14* | 3* | 5 |
| | 0* | 162 | 0* | 8 | 26 | 34 | 0* | 27* | 5* | 8 |
| 1250 | ( 0*) | ( 156 ) | ( 0*) | ( 10 ) | ( 32 ) | ( 35 ) | ( 0*) | ( 21*) | ( 4*) | ( 7 ) |
| | 0* | 150* | 0* | 8* | 50 | 48 | 0* | 18* | 0* | 11* |
| | 0* | 146* | 0* | 9* | 36 | 40 | 0* | 17* | 1* | 6* |
| 2500 | ( 0*) | ( 148*) | ( 0*) | ( 9*) | ( 43 ) | ( 44 ) | ( 0*) | ( 18*) | ( 1*) | ( 9*) |
| | 0* | 120* | 0* | 6* | 29* | 42* | 0* | 0* | 0* | 4* |
| | 0* | 101* | 0* | 6* | 40* | 28* | 0* | 0* | 0* | 4* |
| 5000 | ( 0*) | ( 111*) | ( 0*) | ( 6*) | ( 35*) | ( 35*) | ( 0*) | ( 0*) | ( 0*) | ( 4*) |
| Judgement | — | — | — | — | — | — | — | — | — | — |
| Specific Mutagenicity | | | | | | | | | | |
| Positive Control | AF2 | 2AA | $NaN_3$ | 2AA | AF2 | 2AA 20 | AF2 | 2AA | 9AA | 2AA |
| | ( 741 ) | (1131 ) | ( 293 ) | ( 196 ) | ( 218 ) | (1097 ) | ( 366 ) | ( 500 ) | ( 390 ) | ( 221 ) |

Experimental Data

| Con. μg/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 | ( 152 ) | ( 184 ) | ( 9 ) | ( 10 ) | ( 40 ) | ( 42 ) | ( 24 ) | ( 28 ) | ( 9 ) | ( 10 ) |
| | 126 | | 5 | | | | | | | |
| | 151 | | 2 | | | | | | | |
| 2.44 | ( 139 ) | | ( 4 ) | | | | | | | |
| | 149 | | 10 | | | | | | | |
| | 157 | | 5 | | | | | | | |
| 4.88 | ( 153 ) | | ( 8 ) | | | | | | | |
| | 138 | | 9 | | | | 20 | | | |
| | 142 | | 5 | | | | 27 | | | |
| 9.77 | ( 140 ) | | ( 7 ) | | | | ( 24 ) | | | |
| | 110 | | 7 | | | | 15 | 30 | 8 | |
| | 117 | | 5 | | | | 26 | 26 | 6 | |
| 19.5 | ( 114 ) | | ( 6 ) | | | | ( 21 ) | ( 28 ) | ( 7 ) | |
| | 72* | 170 | 5 | 9 | 25 | 39 | 22 | 27 | 2 | 11 |
| | 100* | 177 | 9 | 7 | 40 | 34 | 20 | 28 | 5 | 13 |
| 39.1 | ( 86*) | ( 174 ) | ( 7 ) | ( 8 ) | ( 33 ) | ( 37 ) | ( 21 ) | ( 28 ) | ( 4 ) | ( 12 ) |
| | 59* | 155 | 6* | 11 | 33 | 42 | 21 | 28 | 5 | 11 |
| | 81* | 172 | 7* | 12 | 37 | 36 | 24 | 22 | 9 | 12 |
| 78.1 | ( 70*) | ( 164 ) | ( 7*) | ( 12 ) | ( 35 ) | ( 39 ) | ( 23 ) | ( 25 ) | ( 7 ) | ( 12 ) |
| | 58* | 189 | 3* | 11 | 49 | 29 | 21 | 23 | 5 | 9 |
| | 62* | 183 | 0* | 8 | 20 | 42 | 18* | 32 | 5 | 7 |
| 156 | ( 60*) | ( 186 ) | ( 2*) | ( 10 ) | ( 35 ) | ( 36 ) | ( 20*) | ( 28 ) | ( 5 ) | ( 8 ) |
| | 0* | 170 | 0* | 8 | 33 | 32 | 17* | 32 | 11 | 11 |
| | 0* | 176 | 0* | 6 | 30 | 46 | 0* | 29 | 9 | 10 |
| 313 | ( 0*) | ( 173 ) | ( 0*) | ( 7 ) | ( 32 ) | ( 39 ) | ( 9*) | ( 31 ) | ( 10 ) | ( 11 ) |
| | | 149 | | 8 | 33 | 43 | 0* | 34 | 4* | 11 |
| | | 157 | | 6 | 31 | 50 | 0* | 24 | 8* | 10 |
| 625 | | ( 153 ) | | ( 7 ) | ( 32 ) | ( 47 ) | ( 0*) | ( 29 ) | ( 6*) | ( 11 ) |

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Experimental Data

| Con. μg/plate | Number of Revertants/plate | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | Base-substitution | | | | | | Frame-shift | | | |
| | TA100 | | TA1535 | | WP2uvrA | | TA98 | | TA1537 | |
| | S9- | S9+ | S9- | S9+ | S9- | S9+ | S9- | S9+ | S9- | S9+ |
| | | 142 | | 12 | 19 | 36 | 0* | 23 | 1* | 9 |
| | | 159 | | 9 | 35 | 37 | 0* | 33 | 0* | 8 |
| 1250 | | ( 151 ) | | ( 11 ) | ( 27 ) | ( 37 ) | ( 0*) | ( 28 ) | ( 1*) | ( 9 ) |
| | | 89* | | 8 | 25 | 34 | | 27* | 0* | 10 |
| | | 80* | | 10 | 25 | 41 | | 25* | 0* | 7 |
| 2500 | | ( 85*) | | ( 9 ) | ( 25 ) | ( 38 ) | | ( 26*) | ( 0*) | ( 9 ) |
| | | 0* | | 4* | 29 | 16 | | | | 5 |
| | | 0* | | 3* | 23 | 15 | | | | 5 |
| 5000 | | ( 0*) | | ( 4*) | ( 26 ) | ( 16 ) | | | | ( 5 ) |
| Judgement | — | — | — | — | — | — | — | — | — | — |
| Specific Mutagenicity Positive | AF2 | 2AA | $NaN_3$ | 2AA | AF2 | 2AA 20 | AF2 | 2AA | 9AA | 2AA |
| Control | ( 639 ) | ( 966 ) | ( 368 ) | ( 239 ) | ( 244 ) | (1131 ) | ( 333 ) | ( 421 ) | ( 385 ) | ( 162 ) |

| Con. μg/plate | Experimental Data: Number of Revertants/plate, Base-substitution | | | | | |
|---|---|---|---|---|---|---|
| | TA102 | | TA104 | | WP2uvrA/pKM101 | |
| | S9- | S9+ | S9- | S9+ | S9- | S9+ |
| Acetone | ( 230 ) | ( 291 ) | ( 297 ) | ( 261 ) | ( 103 ) | ( 147 ) |
| | | | 276 | | | |
| | | | 239 | | | |
| 1.22 | | | ( 258 ) | | | |
| | 233 | | 279 | | | |
| | 222 | | 266 | | | |
| 2.44 | ( 228 ) | | ( 273 ) | | | |
| | 267 | | 262 | | | |
| | 227 | | 256 | | | |
| 4.88 | ( 247 ) | | ( 259 ) | | | |
| | 259 | | 246 | | | |
| | 259 | | 267 | | | |
| 9.77 | ( 259 ) | | ( 257 ) | | | |
| | 191 | | 246 | | 122 | 146 |
| | 246 | | 272 | | 115 | 121 |
| 19.5 | ( 219 ) | | ( 259 ) | | ( 119 ) | ( 134 ) |
| | 249 | 301 | 223 | 291 | 114 | 159 |
| | 247 | 290 | 239 | 265 | 107 | 138 |
| 39.1 | ( 248 ) | ( 296 ) | ( 231 ) | ( 278 ) | ( 111 ) | ( 149 ) |
| | 216 | 309 | 190* | 275 | 124 | 148 |
| | 197 | 298 | 229* | 285 | 119 | 146 |
| 78.1 | ( 207 ) | ( 304 ) | ( 210*) | ( 280 ) | ( 122 ) | ( 147 ) |
| | 153* | 318 | 84* | 301 | 115 | 128 |
| | 141* | 293 | 57* | 311 | 96 | 152 |
| 156 | ( 147*) | ( 306 ) | ( 71*) | ( 306 ) | ( 106 ) | ( 140 ) |
| | | 336 | | 278 | 101 | 120 |
| | | 305 | | 258 | 108 | 145 |
| 313 | | ( 321 ) | | ( 268 ) | ( 105 ) | ( 133 ) |
| | | 276 | | 271 | 108 | 134 |
| | | 287 | | 269 | 91 | 126 |
| 625 | | ( 282 ) | | ( 270 ) | ( 100) | ( 130 ) |

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Experimental Data

| Con. μg/plate | Number of Revertants/plate | | | | | |
|---|---|---|---|---|---|---|
| | Base-substitution | | | | | |
| | TA102 | | TA104 | | WP2uvrA/pKM101 | |
| | S9- | S9+ | S9- | S9+ | S9- | S9+ |
| | | 186 | | 221 | 76* | 123 |
| | | 173 | | 183 | 78* | 104 |
| 1250 | | ( 180 ) | | ( 202 ) | ( 77*) | ( 114 ) |
| | | 66* | | 221 | | 96* |
| | | 46* | | 183 | | 97* |
| 2500 | | ( 56*) | | ( 202 ) | ( ) | ( 97*) |
| | | 66* | | 0* | | 86* |
| | | 46* | | 0* | | 61* |
| 5000 | | ( 56*) | | ( 0*) | ( ) | ( 74*) |
| Judgement | — | — | — | — | — | — |
| Specific Mutagenicity | | | | | | |
| Positive Control | BLM ( 564 ) | 2AA (1184 ) | PA (1821 ) | 2AA (1396 ) | AF2 ( 671 ) | 2AA ( 635 ) |