| Molecule | RI-CIS(D)/def2-SVP $\Delta E(S_0\text{-}S_1)$ [eV] | $\Delta E(S_0\text{-}T_1)$ [eV] | $\Delta E(S_1\text{-}T_1)$ [eV] | $\Delta E_{(D)}(S_1)$ [eV] | $\Delta E_{(D)}(T_1)$ [eV] |
|---|---|---|---|---|---|
| S1 | 1.0364 | 1.3708 | -0.3344 | -0.7737 | -0.1257 |
| S2 | 0.9312 | 1.2510 | -0.3198 | -0.6390 | 0.1001 |
| S3 | 1.3940 | 1.7153 | -0.3213 | -0.8677 | -0.0820 |
| S4 | 1.5918 | 1.9786 | -0.3868 | -1.0077 | -0.1566 |
| S5 | 1.6146 | 1.7314 | -0.1168 | -0.6868 | 0.2653 |
| S6 | 1.3537 | 1.7037 | -0.3500 | -0.9445 | -0.1090 |
| S7 | 1.7591 | 2.0770 | -0.3179 | -0.9595 | -0.0232 |
| S8 | 1.3223 | 1.6095 | -0.2872 | -0.7294 | 0.1312 |
| S9 | 1.4154 | 1.8893 | -0.4739 | -0.9241 | 0.0755 |
| S10 | 1.9040 | 2.0536 | -0.1496 | -0.8043 | 0.1948 |
| S11 | 1.5231 | 1.9190 | -0.3959 | -1.0457 | -0.1872 |
| S12 | 1.7719 | 2.2031 | -0.4312 | -1.1973 | -0.2813 |
| S13 | 1.8615 | 2.2858 | -0.4243 | -1.1290 | -0.1030 |
| S14 | 1.9999 | 2.5065 | -0.5066 | -1.3337 | -0.2444 |
| S15 | 1.5062 | 1.8726 | -0.3664 | -0.9512 | 0.1058 |
| S16 | 1.8226 | 2.2227 | -0.4001 | -1.0699 | 0.0417 |
| S17 | 1.6224 | 1.9992 | -0.3768 | -1.0793 | -0.1488 |
| S18 | 1.7671 | 2.6917 | -0.9246 | -1.2844 | 0.2247 |
| S19 | 1.3998 | 1.6440 | -0.2442 | -0.7044 | 0.2564 |
| S20 | 1.3997 | 1.7596 | -0.3599 | -0.8998 | 0.1437 |
| S21 | 0.8254 | 1.1078 | -0.2824 | -0.5076 | 0.2115 |
| S22 | 1.3899 | 1.5405 | -0.1506 | -0.5630 | 0.3649 |
| S23 | 1.7676 | 1.6961 | 0.0715 | -0.5272 | 0.4922 |
| S24 | 1.4816 | 1.7221 | -0.2405 | -0.7937 | 0.3254 |
| S25 | 1.7474 | 2.0007 | -0.2533 | -0.8026 | 0.2955 |
| S26 | 1.5004 | 1.8865 | -0.3861 | -0.8788 | 0.1753 |
| S27 | 1.7531 | 2.1219 | -0.3688 | -0.9810 | 0.2272 |
| S28 | 1.6890 | 1.6795 | 0.0095 | -0.5261 | 0.4045 |
| S29 | 1.9927 | 2.0438 | -0.0511 | -0.6454 | 0.4465 |
| S30 | 1.2779 | 1.6466 | -0.3687 | -0.8167 | 0.1445 |
| S31 | 1.5342 | 1.9154 | -0.3812 | -0.9306 | 0.1600 |
| S32 | 2.0183 | 2.1354 | -0.1171 | -0.7909 | 0.3724 |
| S33 | 1.7954 | 2.1431 | -0.3477 | -1.0603 | 0.1444 |
| S34 | 1.3618 | 1.6755 | -0.3137 | -0.8111 | 0.1077 |
| S35 | 2.3059 | 2.1866 | 0.1193 | -0.6301 | 0.5164 |
| S36 | 2.0801 | 2.2359 | -0.1558 | -0.8931 | 0.3454 |
| S37 | 1.5367 | 1.9852 | -0.4485 | -1.1378 | -0.0428 |
| S38 | 1.9931 | 2.3332 | -0.3401 | -1.0097 | 0.3337 |
| S39 | 1.8984 | 2.3792 | -0.4808 | -1.2449 | 0.1442 |
| S40 | 1.2247 | 1.6137 | -0.3890 | -0.9308 | -0.0151 |
| S41 | 1.5453 | 1.9270 | -0.3817 | -1.0107 | 0.0398 |
| S42 | 1.9154 | 2.2119 | -0.2965 | -0.9118 | 0.3397 |
| S43 | 1.7723 | 2.2803 | -0.5080 | -1.1681 | 0.1479 |
| S44 | 1.5041 | 1.9050 | -0.4009 | -1.0587 | -0.2828 |
| S45 | 1.3784 | 1.7242 | -0.3458 | -0.9560 | -0.0254 |
| S46 | 2.0921 | 2.3882 | -0.2961 | -1.0723 | -1.4455 |
| S47 | 1.8363 | 2.3145 | -0.4782 | -1.1547 | -0.1773 |
| S48 | 1.6650 | 2.0627 | -0.3977 | -1.0633 | 0.0104 |
| S49 | 1.7820 | 2.2651 | -0.4831 | -1.0057 | 0.2675 |
| S50 | 1.7561 | 2.1223 | -0.3662 | -1.0516 | -0.0275 |
| S51 | 2.1316 | 2.5987 | -0.4671 | -1.2917 | -0.2247 |
| S52 | 2.0740 | 2.6141 | -0.5401 | -1.2757 | -0.1282 |
| S53 | 2.2707 | 2.8825 | -0.6118 | -1.4949 | -0.3264 |
| S54 | 2.2685 | 2.7222 | -0.4537 | -1.1526 | 0.3151 |
| S55 | 1.8389 | 2.3155 | -0.4766 | -1.2256 | -0.0653 |
| S56 | 2.0713 | 2.6137 | -0.5424 | -1.4228 | 0.2219 |
| S57 | 2.0915 | 2.0705 | 0.0210 | -0.6554 | 0.5386 |
| S58 | 1.1082 | 1.4260 | -0.3178 | -0.8700 | 0.0649 |
| S59 | 1.4989 | 1.8071 | -0.3082 | -0.9901 | 0.1699 |
| S60 | 2.2839 | 2.4609 | -0.1770 | -0.9151 | 0.2985 |
| S61 | 2.1441 | 2.5602 | -0.4161 | -1.1642 | 0.1799 |
| S62 | 2.5914 | 2.5616 | 0.0298 | -0.7595 | 0.5193 |
| S63 | 1.7972 | 2.0516 | -0.2544 | -0.8979 | 0.2507 |
| S64 | 2.1488 | 2.4337 | -0.2849 | -1.0338 | 0.2790 |
| S65 | 1.6880 | 2.1350 | -0.4470 | -1.2975 | -0.2423 |
| S66 | 1.6875 | 2.0581 | -0.3706 | -0.9069 | 0.3183 |
| S67 | 1.6105 | 2.0439 | -0.4334 | -1.1909 | -0.0602 |
| S68 | 1.9571 | 2.3565 | -0.3994 | -1.2060 | -0.0890 |
| S69 | 1.9754 | 2.6360 | -0.6606 | -1.4397 | 0.2293 |
| S70 | 2.2663 | 2.5850 | -0.3187 | -1.0223 | 0.3550 |
| S71 | 1.5976 | 2.0575 | -0.4599 | -1.1791 | -0.1345 |
| S72 | 1.8427 | 2.4622 | -0.6195 | -1.3508 | 0.1819 |
| S73 | 1.9798 | 2.4804 | -0.5006 | -1.3632 | -0.4443 |
| S74 | 1.8373 | 2.4018 | -0.5645 | -1.2722 | -0.0277 |
| S75 | 1.3911 | 1.7046 | -0.3135 | -0.7649 | 0.2276 |
| S76 | 1.9555 | 2.1753 | -0.2198 | -0.8753 | 0.4808 |
| S77 | 1.9799 | 2.4485 | -0.4686 | -1.1132 | 0.2919 |
| S78 | 1.7916 | 2.1926 | -0.4010 | -0.9015 | 0.3318 |
| S79 | 1.7564 | 2.2279 | -0.4715 | -1.0772 | 0.2362 |
| S80 | 2.4476 | 2.7382 | -0.2906 | -1.0183 | 0.5016 |
| S81 | 2.2297 | 2.8405 | -0.6108 | -1.3753 | 0.2339 |

| Molecule | RI-CIS(D)/def2-SVP $\Delta E(S_0\text{-}S_1)$ [eV] | $\Delta E(S_0\text{-}T_1)$ [eV] | $\Delta E(S_1\text{-}T_1)$ [eV] | $\Delta E_{(D)}(S_1)$ [eV] | $\Delta E_{(D)}(T_1)$ [eV] |
|---|---|---|---|---|---|
| S82 | 1.6552 | 2.1699 | -0.5147 | -1.1876 | -0.0779 |
| S83 | 2.1985 | 2.5851 | -0.3866 | -1.2662 | 0.2136 |
| S84 | 2.4635 | 3.0462 | -0.5827 | -1.7290 | -1.8602 |
| S85 | 2.1885 | 2.5209 | -0.3324 | -1.6516 | 0.2257 |
| S86 | 1.6218 | 2.0228 | -0.4010 | -1.1890 | 0.1174 |
| S87 | 2.0250 | 2.4757 | -0.4507 | -1.3121 | 0.1722 |
| S88 | 1.9442 | 2.3634 | -0.4192 | -1.5864 | 0.1832 |
| S89 | 0.7160 | 0.9676 | -0.2516 | -0.3754 | 0.2955 |
| S90 | 1.8821 | 1.6648 | 0.2173 | -0.3902 | 0.5963 |
| S91 | 1.0888 | 1.4196 | -0.3308 | -0.7916 | 0.1575 |
| S92 | 2.4302 | 2.1662 | 0.2640 | -0.5119 | 0.6595 |
| S93 | 1.1577 | 1.4857 | -0.3280 | -0.7029 | 0.1907 |
| S94 | 1.9749 | 2.1113 | -0.1364 | -0.7283 | 0.5260 |
| S95 | 1.9791 | 2.1164 | -0.1373 | -0.7535 | 0.5245 |
| S96 | 1.5014 | 1.9920 | -0.4906 | -1.0406 | 0.1157 |
| S97 | 1.0273 | 1.3376 | -0.3103 | -0.7430 | 0.1006 |
| S98 | 2.9600 | 2.7028 | 0.2572 | -0.6171 | -0.9710 |
| S99 | 1.9156 | 1.9835 | -0.0679 | -0.7701 | 0.4481 |
| S100 | 1.3631 | 1.8081 | -0.4450 | -1.1226 | -0.1025 |
| S101 | 2.6173 | 2.6858 | -0.0685 | -0.8484 | 0.6020 |
| S102 | 1.4381 | 1.9167 | -0.4786 | -1.1301 | 0.0772 |
| S103 | 2.2062 | 2.3939 | -0.1877 | -1.1324 | 0.1607 |
| S104 | 1.7118 | 2.3125 | -0.6007 | -1.5240 | -2.0022 |
| S105 | 1.0761 | 1.4213 | -0.3452 | -0.8184 | -0.1628 |
| S106 | 1.1085 | 1.4116 | -0.3031 | -0.7288 | -0.0685 |
| S107 | 1.3119 | 1.6657 | -0.3538 | -0.8762 | -0.1437 |
| S108 | 1.1940 | 1.3750 | -0.1810 | -0.6105 | 0.1033 |
| S109 | 1.2685 | 1.6216 | -0.3531 | -0.8499 | -0.1439 |
| S110 | 1.1958 | 1.3495 | -0.1537 | -0.5926 | 0.1359 |
| S111 | 1.1836 | 1.5363 | -0.3527 | -0.8068 | -0.1372 |
| S112 | 1.0376 | 1.3080 | -0.2704 | -0.7078 | -0.0259 |
| S113 | 1.1181 | 1.4685 | -0.3504 | -0.8091 | -0.1507 |
| S114 | 1.0145 | 1.3166 | -0.3021 | -0.7384 | -0.0793 |
| S115 | 1.0761 | 1.4172 | -0.3411 | -0.7762 | -0.1237 |
| S116 | 0.9988 | 1.3318 | -0.3330 | -0.7792 | -0.1291 |
| S117 | 1.0549 | 1.3910 | -0.3361 | -0.7650 | -0.1134 |
| S118 | 1.0105 | 1.3485 | -0.3380 | -0.7922 | -0.1419 |
| S119 | 1.3520 | 1.6937 | -0.3417 | -0.8730 | -0.1289 |
| S120 | 1.0414 | 1.3379 | -0.2965 | -0.7082 | -0.0436 |
| S121 | 0.9931 | 1.2942 | -0.3011 | -0.7879 | -0.1411 |
| S122 | 1.0601 | 1.3881 | -0.3280 | -0.7635 | -0.1273 |
| S123 | 0.8810 | 1.1206 | -0.2396 | -0.6722 | 0.0074 |
| S124 | 1.3535 | 1.6770 | -0.3235 | -0.7887 | -0.0698 |
| S125 | 0.9343 | 1.2425 | -0.3082 | -0.7426 | -0.0975 |
| S126 | 1.1005 | 1.4326 | -0.3321 | -0.7990 | -0.1427 |
| S127 | 0.9688 | 1.2848 | -0.3160 | -0.7938 | -0.1546 |
| S128 | 1.0893 | 1.4184 | -0.3291 | -0.7485 | -0.1051 |
| S129 | 0.9134 | 1.1964 | -0.2830 | -0.6772 | 0.0071 |
| S130 | 1.2131 | 1.5411 | -0.3280 | -0.8102 | -0.1072 |
| S131 | 1.3411 | 1.6865 | -0.3454 | -0.8688 | -0.1331 |
| S132 | 1.0107 | 1.3403 | -0.3296 | -0.7470 | -0.1005 |
| S133 | 0.8562 | 1.1261 | -0.2699 | -0.7016 | -0.0354 |
| S134 | 1.3351 | 1.6526 | -0.3175 | -0.7798 | -0.0611 |
| S135 | 1.0182 | 1.3247 | -0.3065 | -0.7365 | -0.0781 |
| S136 | 1.1158 | 1.4616 | -0.3458 | -0.8185 | -0.1603 |
| S137 | 0.8788 | 1.1289 | -0.2501 | -0.5899 | 0.1286 |
| S138 | 1.4216 | 1.7633 | -0.3417 | -0.8144 | -0.0061 |
| S139 | 0.9640 | 1.2718 | -0.3078 | -0.7191 | -0.0505 |
| S140 | 1.1752 | 1.5146 | -0.3394 | -0.8055 | -0.1307 |
| S141 | 2.5172 | 3.1198 | -0.6026 | -1.7698 | -0.8089 |
| S142 | 2.8711 | 3.4184 | -0.5473 | -1.7682 | -0.6607 |
| S143 | 2.7720 | 3.3634 | -0.5914 | -1.7694 | -0.7124 |
| S144 | 2.6720 | 3.2742 | -0.6022 | -1.7486 | -0.7639 |
| S145 | 2.5894 | 3.1979 | -0.6085 | -1.7580 | -0.7887 |
| S146 | 2.5364 | 3.1282 | -0.5918 | -1.7420 | -0.8039 |
| S147 | 2.5081 | 3.0947 | -0.5866 | -1.7385 | -0.8053 |
| S148 | 2.9014 | 3.4333 | -0.5319 | -1.7621 | -0.6478 |
| S149 | 2.4505 | 3.8347 | -1.3842 | -1.7756 | 0.7790 |
| S150 | 2.3390 | 3.0447 | -0.7057 | -1.6830 | -0.2345 |
| S151 | 2.3889 | 2.9506 | -0.5617 | -1.7296 | -0.8074 |
| S152 | 2.4440 | 3.0151 | -0.5711 | -1.7719 | -0.8532 |
| S153 | 2.3652 | 2.9370 | -0.5718 | -1.6776 | -0.6512 |
| S154 | 2.9107 | 3.4391 | -0.5284 | -1.7591 | -0.6429 |
| S155 | 2.3500 | 3.0520 | -0.7020 | -1.7001 | -0.4125 |
| S156 | 2.4604 | 3.0378 | -0.5774 | -1.7465 | -0.8096 |
| S157 | 2.4743 | 3.8700 | -1.3957 | -1.7021 | 1.4650 |
| S158 | 2.4154 | 2.9974 | -0.5820 | -1.7112 | -0.7262 |
| S159 | 1.5676 | 1.9693 | -0.4017 | -1.0948 | -0.2645 |
| S160 | 1.5769 | 1.9802 | -0.4033 | -1.0804 | -0.1913 |
| S161 | 1.5485 | 1.9354 | -0.3869 | -1.0057 | -0.1298 |
| S162 | 1.5298 | 1.9107 | -0.3809 | -1.0226 | -0.1673 |

| Molecule | RI-CIS(D)/def2-SVP $\Delta E(S_0\text{-}S_1)$ [eV] | $\Delta E(S_0\text{-}T_1)$ [eV] | $\Delta E(S_1\text{-}T_1)$ [eV] | $\Delta E_{(D)}(S_1)$ [eV] | $\Delta E_{(D)}(T_1)$ [eV] |
|---|---|---|---|---|---|
| S163 | 1.8426 | 2.2750 | -0.4324 | -1.1649 | -0.3249 |
| S164 | 1.8662 | 2.2048 | -0.3386 | -1.0838 | -0.0721 |
| S165 | 1.4946 | 1.8142 | -0.3196 | -0.9251 | 0.0267 |
| S166 | 1.4548 | 1.7948 | -0.3400 | -0.9749 | -0.0901 |
| S167 | 1.7663 | 2.2009 | -0.4346 | -1.1375 | -0.3147 |
| S168 | 1.8240 | 2.1731 | -0.3491 | -1.0615 | -0.0732 |
| S169 | 1.4671 | 1.8142 | -0.3471 | -0.9792 | -0.0680 |
| S170 | 1.4566 | 1.7833 | -0.3267 | -0.9608 | -0.0431 |
| S171 | 1.6640 | 2.0985 | -0.4345 | -1.0930 | -0.2677 |
| S172 | 1.7162 | 2.0992 | -0.3830 | -1.0466 | -0.1250 |
| S173 | 1.4219 | 1.7867 | -0.3648 | -1.0210 | -0.1263 |
| S174 | 1.4401 | 1.8118 | -0.3717 | -1.0264 | -0.1411 |
| S175 | 1.6023 | 2.0181 | -0.4158 | -1.0916 | -0.2666 |
| S176 | 1.6349 | 2.0328 | -0.3979 | -1.0568 | -0.1512 |
| S177 | 1.5273 | 1.9311 | -0.4038 | -1.0791 | -0.2355 |
| S178 | 1.5617 | 1.9738 | -0.4121 | -1.0734 | -0.1995 |
| S179 | 1.5484 | 1.9591 | -0.4107 | -1.0590 | -0.2082 |
| S180 | 1.5923 | 1.9850 | -0.3927 | -1.0357 | -0.1617 |
| S181 | 1.4465 | 1.8386 | -0.3921 | -1.0604 | -0.1998 |
| S182 | 1.4703 | 1.8712 | -0.4009 | -1.0610 | -0.1957 |
| S183 | 1.5253 | 1.9294 | -0.4041 | -1.0471 | -0.1861 |
| S184 | 1.5699 | 1.9592 | -0.3893 | -1.0288 | -0.1653 |
| S185 | 1.4563 | 1.8531 | -0.3968 | -1.0739 | -0.2194 |
| S186 | 1.4828 | 1.8904 | -0.4076 | -1.0724 | -0.2046 |
| S187 | 1.8890 | 2.3155 | -0.4265 | -1.1639 | -0.3119 |
| S188 | 1.9310 | 2.2328 | -0.3018 | -1.0693 | -0.0363 |
| S189 | 1.4794 | 1.8485 | -0.3691 | -0.9856 | -0.0875 |
| S190 | 1.4877 | 1.8055 | -0.3178 | -0.9657 | -0.0742 |
| S191 | 1.4438 | 1.8013 | -0.3575 | -1.0785 | -0.2483 |
| S192 | 1.5130 | 1.9152 | -0.4022 | -1.0674 | -0.1808 |
| S193 | 1.4990 | 1.8863 | -0.3873 | -1.0230 | -0.1702 |
| S194 | 1.4981 | 1.8918 | -0.3937 | -1.0338 | -0.1944 |
| S195 | 1.3103 | 1.6042 | -0.2939 | -0.9543 | -0.0373 |
| S196 | 1.4324 | 1.7739 | -0.3415 | -0.9746 | -0.0887 |
| S197 | 1.6334 | 2.0407 | -0.4073 | -1.1212 | -0.2500 |
| S198 | 1.6710 | 2.0936 | -0.4226 | -1.0938 | -0.1874 |
| S199 | 1.4083 | 1.7630 | -0.3547 | -1.0201 | -0.1498 |
| S200 | 1.4488 | 1.8281 | -0.3793 | -1.0166 | -0.1705 |
| S201 | 1.5154 | 1.9106 | -0.3952 | -1.0769 | -0.2351 |
| S202 | 1.5469 | 1.9569 | -0.4100 | -1.0680 | -0.2105 |
| S203 | 1.4236 | 1.7890 | -0.3654 | -1.0842 | -0.2436 |
| S204 | 1.4972 | 1.8847 | -0.3875 | -1.0569 | -0.2044 |
| S205 | 1.5121 | 1.9074 | -0.3953 | -1.0259 | -0.1720 |
| S206 | 1.5472 | 1.9499 | -0.4027 | -1.0249 | -0.1751 |
| S207 | 1.3611 | 1.6894 | -0.3283 | -0.9572 | -0.0237 |
| S208 | 1.4496 | 1.8051 | -0.3555 | -0.9621 | -0.0771 |
| S209 | 1.5784 | 1.9886 | -0.4102 | -1.1114 | -0.2383 |
| S210 | 1.6504 | 2.0695 | -0.4191 | -1.0820 | -0.1945 |
| S211 | 1.8731 | 2.2965 | -0.4234 | -1.1525 | -0.3104 |
| S212 | 1.8986 | 2.2222 | -0.3236 | -1.0760 | -0.0649 |
| S213 | 1.4931 | 1.8649 | -0.3718 | -0.9977 | -0.1061 |
| S214 | 1.4878 | 1.8629 | -0.3751 | -1.0173 | -0.1541 |
| S215 | 1.3260 | 1.6352 | -0.3092 | -0.9713 | -0.0585 |
| S216 | 1.4013 | 1.7512 | -0.3499 | -0.9784 | -0.1081 |
| S217 | 1.6514 | 2.0437 | -0.3923 | -1.0850 | -0.2149 |
| S218 | 1.7595 | 2.1733 | -0.4138 | -1.0412 | -0.1319 |
| S219 | 1.4680 | 1.8421 | -0.3741 | -1.0237 | -0.1405 |
| S220 | 1.5420 | 1.9141 | -0.3721 | -1.0120 | -0.1426 |
| S221 | 1.5582 | 1.9714 | -0.4132 | -1.1012 | -0.2623 |
| S222 | 1.5690 | 1.9953 | -0.4263 | -1.0965 | -0.2116 |
| S223 | 1.3333 | 1.6281 | -0.2948 | -0.8582 | 0.1212 |
| S224 | 1.4602 | 1.8112 | -0.3510 | -0.9056 | -0.0015 |
| S225 | 1.7005 | 2.1323 | -0.4318 | -1.1310 | -0.1784 |
| S226 | 1.8055 | 2.2459 | -0.4404 | -1.0766 | -0.1140 |
| S227 | 1.4213 | 1.7855 | -0.3642 | -1.0004 | -0.0835 |
| S228 | 1.5043 | 1.8771 | -0.3728 | -1.0054 | -0.1247 |
| S229 | 1.5827 | 1.9983 | -0.4156 | -1.1001 | -0.2433 |
| S230 | 1.6559 | 2.0761 | -0.4202 | -1.0729 | -0.1736 |
| S231 | 1.8986 | 2.3397 | -0.4411 | -1.1793 | -0.1709 |
| S232 | 1.9171 | 2.3441 | -0.4270 | -1.1597 | -0.1248 |
| S233 | 1.9033 | 2.3384 | -0.4351 | -1.1639 | -0.0888 |
| S234 | 1.8304 | 2.2516 | -0.4212 | -1.1012 | -0.0743 |
| S235 | 1.9145 | 2.3165 | -0.4020 | -1.0691 | -0.0007 |
| S236 | 1.9019 | 2.3020 | -0.4001 | -1.0918 | -0.0458 |
| S237 | 2.1686 | 2.6639 | -0.4953 | -1.2562 | -0.1692 |
| S238 | 2.1381 | 2.5167 | -0.3786 | -1.1936 | -0.0633 |
| S239 | 2.2323 | 2.5264 | -0.2941 | -1.1380 | 0.0095 |
| S240 | 1.6930 | 2.0523 | -0.3593 | -1.0411 | 0.0423 |
| S241 | 1.8664 | 2.1142 | -0.2478 | -0.9310 | 0.2300 |
| S242 | 1.8545 | 2.1814 | -0.3269 | -1.0293 | 0.0810 |
| S243 | 2.1034 | 2.5953 | -0.4919 | -1.2207 | -0.1520 |

| Molecule | RI-CIS(D)/def2-SVP $\Delta E(S_0\text{-}S_1)$ [eV] | $\Delta E(S_0\text{-}T_1)$ [eV] | $\Delta E(S_1\text{-}T_1)$ [eV] | $\Delta E_{(D)}(S_1)$ [eV] | $\Delta E_{(D)}(T_1)$ [eV] |
|---|---|---|---|---|---|
| S244 | 2.0534 | 2.4731 | -0.4197 | -1.1811 | -0.0823 |
| S245 | 2.1797 | 2.5099 | -0.3302 | -1.1212 | 0.0116 |
| S246 | 1.6681 | 2.0200 | -0.3519 | -1.0537 | 0.0348 |
| S247 | 1.8978 | 2.1855 | -0.2877 | -0.9864 | 0.1470 |
| S248 | 1.8794 | 2.1849 | -0.3055 | -1.0150 | 0.1280 |
| S249 | 1.9887 | 2.4641 | -0.4754 | -1.1861 | -0.1752 |
| S250 | 1.9678 | 2.4241 | -0.4563 | -1.1658 | -0.1152 |
| S251 | 2.0888 | 2.4581 | -0.3693 | -1.1092 | -0.0295 |
| S252 | 1.7052 | 2.1009 | -0.3957 | -1.1261 | -0.0779 |
| S253 | 1.8474 | 2.2123 | -0.3649 | -1.0861 | 0.0200 |
| S254 | 1.7891 | 2.1734 | -0.3843 | -1.1029 | -0.0439 |
| S255 | 1.9411 | 2.3992 | -0.4581 | -1.1776 | -0.1708 |
| S256 | 1.9092 | 2.3464 | -0.4372 | -1.1565 | -0.1309 |
| S257 | 1.9874 | 2.3987 | -0.4113 | -1.1333 | -0.0514 |
| S258 | 1.7172 | 2.1125 | -0.3953 | -1.1180 | -0.0904 |
| S259 | 1.8115 | 2.1626 | -0.3511 | -1.0745 | -0.0180 |
| S260 | 1.8833 | 2.3360 | -0.4527 | -1.1611 | -0.1131 |
| S261 | 1.8831 | 2.3266 | -0.4435 | -1.1489 | -0.1331 |
| S262 | 1.8724 | 2.3142 | -0.4418 | -1.1390 | -0.1185 |
| S263 | 1.7599 | 2.1793 | -0.4194 | -1.1544 | -0.1341 |
| S264 | 1.7875 | 2.1967 | -0.4092 | -1.1423 | -0.1167 |
| S265 | 1.8267 | 2.2467 | -0.4200 | -1.1359 | -0.0715 |
| S266 | 1.9528 | 2.3627 | -0.4099 | -1.1174 | -0.0737 |
| S267 | 1.8620 | 2.2970 | -0.4350 | -1.1364 | -0.1134 |
| S268 | 1.8526 | 2.2890 | -0.4364 | -1.1293 | -0.1132 |
| S269 | 1.9270 | 2.3395 | -0.4125 | -1.1163 | -0.0841 |
| S270 | 1.7725 | 2.1977 | -0.4252 | -1.1679 | -0.1519 |
| S271 | 1.7918 | 2.2073 | -0.4155 | -1.1588 | -0.1415 |
| S272 | 1.8275 | 2.2608 | -0.4333 | -1.1519 | -0.0903 |
| S273 | 2.2259 | 2.7166 | -0.4907 | -1.2463 | -0.1139 |
| S274 | 2.1532 | 2.5121 | -0.3589 | -1.1855 | -0.0433 |
| S275 | 2.2723 | 2.5413 | -0.2690 | -1.1241 | 0.0325 |
| S276 | 1.6867 | 2.0347 | -0.3480 | -1.0430 | 0.0395 |
| S277 | 1.9248 | 2.1213 | -0.1965 | -0.9008 | 0.2800 |
| S278 | 1.8558 | 2.2324 | -0.3766 | -1.0658 | 0.0084 |
| S279 | 1.8129 | 2.2226 | -0.4097 | -1.1560 | -0.1421 |
| S280 | 1.8801 | 2.3123 | -0.4322 | -1.1202 | 0.0173 |
| S281 | 1.7971 | 2.2691 | -0.4720 | -1.1844 | -0.1416 |
| S282 | 1.8166 | 2.2287 | -0.4121 | -1.1043 | -0.1012 |
| S283 | 1.7735 | 2.1927 | -0.4192 | -1.0912 | 0.0052 |
| S284 | 1.8253 | 2.2520 | -0.4267 | -1.1119 | -0.0834 |
| S285 | 1.6454 | 1.9669 | -0.3215 | -1.0474 | 0.0139 |
| S286 | 1.8420 | 2.1593 | -0.3173 | -1.0251 | 0.1031 |
| S287 | 1.6956 | 2.0922 | -0.3966 | -1.1069 | -0.2025 |
| S288 | 1.9500 | 2.4132 | -0.4632 | -1.2161 | -0.1966 |
| S289 | 1.8616 | 2.3973 | -0.5357 | -1.2373 | -0.1886 |
| S290 | 1.8839 | 2.3159 | -0.4320 | -1.2049 | -0.1697 |
| S291 | 1.7573 | 2.1391 | -0.3818 | -1.1064 | -0.0879 |
| S292 | 1.8155 | 2.2006 | -0.3851 | -1.0726 | 0.0035 |
| S293 | 1.7682 | 2.2054 | -0.4372 | -1.1314 | -0.1488 |
| S294 | 1.8323 | 2.2606 | -0.4283 | -1.1658 | -0.1787 |
| S295 | 1.8030 | 2.2198 | -0.4168 | -1.1550 | -0.1236 |
| S296 | 1.8297 | 2.2809 | -0.4512 | -1.1656 | -0.1545 |
| S297 | 1.7652 | 2.1623 | -0.3971 | -1.1753 | -0.1833 |
| S298 | 1.8251 | 2.2279 | -0.4028 | -1.1355 | -0.0990 |
| S299 | 1.8548 | 2.2897 | -0.4349 | -1.1469 | -0.1201 |
| S300 | 1.8257 | 2.2559 | -0.4302 | -1.1180 | -0.1092 |
| S301 | 1.8208 | 2.2257 | -0.4049 | -1.1079 | -0.0903 |
| S302 | 1.8569 | 2.3012 | -0.4443 | -1.1170 | -0.0751 |
| S303 | 1.7083 | 2.0567 | -0.3484 | -1.0496 | 0.0264 |
| S304 | 1.8315 | 2.1813 | -0.3498 | -1.0209 | 0.1221 |
| S305 | 1.7689 | 2.1475 | -0.3786 | -1.0734 | -0.1541 |
| S306 | 1.8906 | 2.3344 | -0.4438 | -1.2117 | -0.2137 |
| S307 | 1.8366 | 2.2718 | -0.4352 | -1.2142 | -0.1829 |
| S308 | 1.8868 | 2.3973 | -0.5105 | -1.2074 | -0.1498 |
| S309 | 2.1944 | 2.6796 | -0.4852 | -1.2415 | -0.1512 |
| S310 | 2.1529 | 2.5172 | -0.3643 | -1.1793 | -0.0630 |
| S311 | 2.2565 | 2.5411 | -0.2846 | -1.1330 | 0.0154 |
| S312 | 1.7697 | 2.1659 | -0.3962 | -1.0972 | -0.0676 |
| S313 | 1.8561 | 2.1787 | -0.3226 | -1.0223 | 0.0888 |
| S314 | 1.8718 | 2.2513 | -0.3795 | -1.0770 | -0.0039 |
| S315 | 1.6763 | 2.0126 | -0.3363 | -1.0589 | 0.0063 |
| S316 | 1.7844 | 2.1170 | -0.3326 | -1.0264 | 0.0896 |
| S317 | 1.7099 | 2.1243 | -0.4144 | -1.1244 | -0.1967 |
| S318 | 1.9435 | 2.3748 | -0.4313 | -1.1872 | -0.2117 |
| S319 | 1.9822 | 2.5052 | -0.5230 | -1.1665 | -0.0690 |
| S320 | 1.8576 | 2.2870 | -0.4294 | -1.1968 | -0.1686 |
| S321 | 1.7858 | 2.1841 | -0.3983 | -1.1170 | -0.0915 |
| S322 | 1.8946 | 2.2935 | -0.3989 | -1.0796 | -0.0039 |
| S323 | 1.8919 | 2.3027 | -0.4108 | -1.1217 | -0.1014 |
| S324 | 1.8618 | 2.3171 | -0.4553 | -1.2007 | -0.1908 |

| | RI-CIS(D)/def2-SVP | | | | |
|---|---|---|---|---|---|
| **Molecule** | **$\Delta E(S_0\text{-}S_1)$ [eV]** | **$\Delta E(S_0\text{-}T_1)$ [eV]** | **$\Delta E(S_1\text{-}T_1)$ [eV]** | **$\Delta E_{(D)}(S_1)$ [eV]** | **$\Delta E_{(D)}(T_1)$ [eV]** |
| S325 | 1.8794 | 2.3579 | -0.4785 | -1.1934 | -0.1359 |
| S326 | 1.9111 | 2.3431 | -0.4320 | -1.1757 | -0.1625 |
| S327 | 1.6909 | 2.0237 | -0.3328 | -0.9506 | 0.1943 |
| S328 | 1.8283 | 2.1803 | -0.3520 | -0.9699 | 0.1919 |
| S329 | 1.8829 | 2.2822 | -0.3993 | -1.0620 | -0.0818 |
| S330 | 1.9783 | 2.4574 | -0.4791 | -1.2432 | -0.2008 |
| S331 | 1.9761 | 2.6223 | -0.6462 | -1.2322 | 0.0133 |
| S332 | 1.8716 | 2.3527 | -0.4811 | -1.2503 | -0.1783 |
| S333 | 1.7699 | 2.1557 | -0.3858 | -1.0898 | -0.0213 |
| S334 | 1.8843 | 2.2727 | -0.3884 | -1.0766 | 0.0436 |
| S335 | 1.8444 | 2.2423 | -0.3979 | -1.0919 | -0.1084 |
| S336 | 1.8971 | 2.3456 | -0.4485 | -1.1989 | -0.1949 |
| S337 | 1.8881 | 2.3338 | -0.4457 | -1.2016 | -0.1760 |
| S338 | 1.9479 | 2.4436 | -0.4957 | -1.1788 | -0.0840 |
| S339 | 2.1155 | 2.6503 | -0.5348 | -1.3270 | -0.2511 |
| S340 | 2.1358 | 2.6786 | -0.5428 | -1.3026 | -0.1082 |
| S341 | 2.0732 | 2.6016 | -0.5284 | -1.2253 | -0.0346 |
| S342 | 2.3767 | 2.8699 | -0.4932 | -1.4279 | -0.5025 |
| S343 | 2.4702 | 2.8527 | -0.3825 | -1.2675 | 0.0053 |
| S344 | 1.9280 | 2.2902 | -0.3622 | -1.0966 | 0.2102 |
| S345 | 2.2847 | 2.8197 | -0.5350 | -1.3983 | -0.4401 |
| S346 | 2.3965 | 2.8359 | -0.4394 | -1.2615 | -0.0032 |
| S347 | 1.9235 | 2.3573 | -0.4338 | -1.1723 | 0.1109 |
| S348 | 2.1905 | 2.7691 | -0.5786 | -1.3516 | -0.3086 |
| S349 | 2.3009 | 2.8009 | -0.5000 | -1.2581 | -0.0335 |
| S350 | 1.9455 | 2.4454 | -0.4999 | -1.2677 | -0.0671 |
| S351 | 2.1522 | 2.7061 | -0.5539 | -1.3331 | -0.2753 |
| S352 | 2.1961 | 2.7254 | -0.5293 | -1.2787 | -0.0713 |
| S353 | 1.9461 | 2.4138 | -0.4677 | -1.2402 | -0.0555 |
| S354 | 2.0979 | 2.6602 | -0.5623 | -1.3019 | -0.1737 |
| S355 | 1.9693 | 2.4893 | -0.5200 | -1.3003 | -0.1506 |
| S356 | 2.1583 | 2.6958 | -0.5375 | -1.2675 | -0.0867 |
| S357 | 2.0792 | 2.6348 | -0.5556 | -1.2869 | -0.1367 |
| S358 | 2.1301 | 2.6688 | -0.5387 | -1.2666 | -0.0991 |
| S359 | 1.9771 | 2.5022 | -0.5251 | -1.3175 | -0.1806 |
| S360 | 2.4053 | 2.8924 | -0.4871 | -1.4245 | -0.4920 |
| S361 | 2.4958 | 2.8660 | -0.3702 | -1.2636 | 0.0023 |
| S362 | 1.9001 | 2.3056 | -0.4055 | -1.1602 | 0.0957 |
| S363 | 2.0264 | 2.5176 | -0.4912 | -1.2972 | -0.2003 |
| S364 | 2.0158 | 2.6108 | -0.5950 | -1.3263 | -0.1331 |
| S365 | 2.0135 | 2.5518 | -0.5383 | -1.2398 | -0.0542 |
| S366 | 1.9211 | 2.3215 | -0.4004 | -1.1655 | 0.0540 |
| S367 | 1.9206 | 2.3900 | -0.4694 | -1.2377 | -0.2066 |
| S368 | 2.0908 | 2.6467 | -0.5559 | -1.3776 | -0.2665 |
| S369 | 1.9968 | 2.4763 | -0.4795 | -1.2413 | -0.0825 |
| S370 | 1.9821 | 2.5100 | -0.5279 | -1.2737 | -0.1770 |
| S371 | 2.0011 | 2.5252 | -0.5241 | -1.3067 | -0.1889 |
| S372 | 1.9953 | 2.4910 | -0.4957 | -1.3215 | -0.2072 |
| S373 | 2.0589 | 2.6103 | -0.5514 | -1.2968 | -0.1348 |
| S374 | 2.0161 | 2.5470 | -0.5309 | -1.2611 | -0.1155 |
| S375 | 1.9532 | 2.3992 | -0.4460 | -1.1854 | 0.0621 |
| S376 | 1.9733 | 2.4470 | -0.4737 | -1.2195 | -0.1548 |
| S377 | 2.0512 | 2.6094 | -0.5582 | -1.3745 | -0.2381 |
| S378 | 2.3988 | 2.8807 | -0.4819 | -1.4083 | -0.4816 |
| S379 | 2.4977 | 2.8596 | -0.3619 | -1.2600 | 0.0106 |
| S380 | 1.9370 | 2.3624 | -0.4254 | -1.1953 | 0.0378 |
| S381 | 1.9382 | 2.3556 | -0.4174 | -1.1782 | 0.0383 |
| S382 | 1.9410 | 2.4247 | -0.4837 | -1.2488 | -0.1949 |
| S383 | 2.1020 | 2.6688 | -0.5668 | -1.3803 | -0.2831 |
| S384 | 2.0289 | 2.5496 | -0.5207 | -1.2620 | -0.0744 |
| S385 | 2.1064 | 2.6274 | -0.5210 | -1.2558 | -0.0963 |
| S386 | 2.0854 | 2.6377 | -0.5523 | -1.3455 | -0.2366 |
| S387 | 1.9524 | 2.5329 | -0.5805 | -1.0794 | 0.4309 |
| S388 | 2.0822 | 3.8225 | -1.7403 | -1.2150 | 1.4350 |
| S389 | 2.0871 | 3.8150 | -1.7279 | -1.4151 | 1.1128 |
| S390 | 1.9966 | 2.4958 | -0.4992 | -1.2336 | 0.0046 |
| S391 | 2.0462 | 2.5592 | -0.5130 | -1.2456 | -0.1158 |
| S392 | 2.0944 | 2.6628 | -0.5684 | -1.3637 | -0.2316 |
| S393 | 2.0602 | 2.5769 | -0.5167 | -1.3716 | -0.2726 |
| S394 | 2.0451 | 2.5537 | -0.5086 | -1.3648 | -0.2269 |
| S395 | 1.9960 | 2.4841 | -0.4881 | -1.2949 | -0.1839 |
| S396 | 2.4076 | 2.8926 | -0.4850 | -1.3887 | -0.1395 |
| S397 | 2.3562 | 2.7108 | -0.3546 | -1.3419 | -0.1440 |
| S398 | 1.8723 | 2.2772 | -0.4049 | -1.2352 | -0.0435 |
| S399 | 2.3039 | 2.8212 | -0.5173 | -1.3723 | -0.1641 |
| S400 | 2.2879 | 2.6942 | -0.4063 | -1.3367 | -0.1501 |
| S401 | 1.8702 | 2.2663 | -0.3961 | -1.2404 | -0.0274 |
| S402 | 2.1781 | 2.7210 | -0.5429 | -1.3599 | -0.2306 |
| S403 | 2.2127 | 2.6595 | -0.4468 | -1.3180 | -0.1640 |
| S404 | 1.8766 | 2.3327 | -0.4561 | -1.3240 | -0.1795 |
| S405 | 2.1106 | 2.6349 | -0.5243 | -1.3531 | -0.2371 |

| | RI-CIS(D)/def2-SVP | | | | |
|---|---|---|---|---|---|
| **Molecule** | **$\Delta E(S_0\text{-}S_1)$ [eV]** | **$\Delta E(S_0\text{-}T_1)$ [eV]** | **$\Delta E(S_1\text{-}T_1)$ [eV]** | **$\Delta E_{(D)}(S_1)$ [eV]** | **$\Delta E_{(D)}(T_1)$ [eV]** |
| S406 | 2.1181 | 2.6073 | -0.4892 | -1.3434 | -0.1974 |
| S407 | 1.9967 | 2.5138 | -0.5171 | -1.3723 | -0.3024 |
| S408 | 2.0509 | 2.5709 | -0.5200 | -1.3370 | -0.2424 |
| S409 | 1.9062 | 2.3950 | -0.4888 | -1.3555 | -0.2646 |
| S410 | 2.0850 | 2.5793 | -0.4943 | -1.3266 | -0.2081 |
| S411 | 2.0268 | 2.5383 | -0.5115 | -1.3271 | -0.2367 |
| S412 | 2.0590 | 2.5584 | -0.4994 | -1.3265 | -0.2194 |
| S413 | 1.9141 | 2.4106 | -0.4965 | -1.3703 | -0.2899 |
| S414 | 2.4445 | 2.9034 | -0.4589 | -1.3742 | -0.1034 |
| S415 | 2.3796 | 2.7197 | -0.3401 | -1.3372 | -0.1389 |
| S416 | 1.9247 | 2.3784 | -0.4537 | -1.2750 | -0.1339 |
| S417 | 1.9927 | 2.6373 | -0.6446 | -1.3494 | -0.0209 |
| S418 | 1.9769 | 2.5208 | -0.5439 | -1.3754 | -0.2487 |
| S419 | 1.9434 | 2.4375 | -0.4941 | -1.2977 | -0.2091 |
| S420 | 1.8739 | 2.2975 | -0.4236 | -1.2608 | -0.1175 |
| S421 | 1.8833 | 2.3723 | -0.4890 | -1.3024 | -0.3094 |
| S422 | 2.0526 | 2.6293 | -0.5767 | -1.4233 | -0.3538 |
| S423 | 1.9216 | 2.3985 | -0.4769 | -1.2950 | -0.1772 |
| S424 | 1.9272 | 2.4539 | -0.5267 | -1.3366 | -0.2787 |
| S425 | 1.9629 | 2.4668 | -0.5039 | -1.3613 | -0.3165 |
| S426 | 1.9472 | 2.4285 | -0.4813 | -1.3584 | -0.2843 |
| S427 | 2.0051 | 2.5306 | -0.5255 | -1.3515 | -0.2385 |
| S428 | 1.9698 | 2.4789 | -0.5091 | -1.3147 | -0.2381 |
| S429 | 1.8935 | 2.3377 | -0.4442 | -1.2470 | -0.0762 |
| S430 | 1.9276 | 2.4032 | -0.4756 | -1.2830 | -0.2848 |
| S431 | 2.0314 | 2.5769 | -0.5455 | -1.4100 | -0.3584 |
| S432 | 2.4256 | 2.8897 | -0.4641 | -1.3716 | -0.1332 |
| S433 | 2.3839 | 2.7239 | -0.3400 | -1.3363 | -0.1381 |
| S434 | 1.9305 | 2.3842 | -0.4537 | -1.2894 | -0.1559 |
| S435 | 1.8691 | 2.2937 | -0.4246 | -1.2462 | -0.0909 |
| S436 | 1.8909 | 2.3965 | -0.5056 | -1.3187 | -0.3024 |
| S437 | 2.1107 | 2.6696 | -0.5589 | -1.3685 | -0.2711 |
| S438 | 1.9996 | 2.4807 | -0.4811 | -1.2977 | -0.1673 |
| S439 | 2.0190 | 2.5250 | -0.5060 | -1.3334 | -0.2379 |
| S440 | 2.0018 | 2.5375 | -0.5357 | -1.4060 | -0.3448 |
| S441 | 1.9091 | 3.2457 | -1.3366 | -1.1814 | 1.0324 |
| S442 | 2.0403 | 3.8656 | -1.8253 | -1.2803 | 1.4323 |
| S443 | 2.1237 | 3.5434 | -1.4197 | -1.4307 | 0.6176 |
| S444 | 1.9503 | 2.4262 | -0.4759 | -1.3009 | -0.1504 |
| S445 | 1.9760 | 2.4721 | -0.4961 | -1.3062 | -0.2547 |
| S446 | 2.0653 | 2.6134 | -0.5481 | -1.3950 | -0.3098 |