Marcos André Lopes Mendes | nº mec: 90706 | Data: 21/10/2020

N-Pentano

Formula Smiles:

```
C-C-C-C-C
```

Formula XYZ :

```
C          1.20735         0.32459         0.30375
C          2.71227         0.38769         0.09686
C          3.35238        -0.99526         0.21457
C          4.86416        -0.92828        -0.00043
C          5.51120        -2.29441         0.16270
H          0.77418         1.32795         0.24424
H          0.96243        -0.09366         1.28511
H          0.73260        -0.29627        -0.46296
H          3.14872         1.06310         0.84218
H          2.92274         0.81447        -0.89047
H          2.90624        -1.67228        -0.52428
H          3.13971        -1.41414         1.20569
H          5.31313        -0.23147         0.71723
H          5.07992        -0.54422        -1.00404
H          5.35110        -2.68566         1.17225
H          6.59019        -2.22548        -0.00750
H          5.09910        -3.01242        -0.55383
```

Energia:

```
C H A R G E S

IDX     CHARGE
1       -0.065276
2       -0.055919
3       -0.053555
4       -0.055919
5       -0.065276
6       0.022978
7       0.022978
8       0.022978
9       0.026265
10      0.026265
11      0.026512
12      0.026512
13      0.026265
14      0.026265
15      0.022978
16      0.022978
17      0.022978

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP IMPROPER TORSION CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

E N E R G Y

     TOTAL BOND STRETCHING ENERGY =    0.847 kJ/mol
     TOTAL ANGLE BENDING ENERGY =    0.955 kJ/mol
     TOTAL TORSIONAL ENERGY =    0.077 kJ/mol
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol
     TOTAL VAN DER WAALS ENERGY =    3.988 kJ/mol
     TOTAL ELECTROSTATIC ENERGY =    1.775 kJ/mol

TOTAL ENERGY =    7.642 kJ/mol
```

Marcos André Lopes Mendes | nº mec: 90706 | Data: 21/10/2020

Isopentano

Formula Smiles:

```
c-C(-C)-C-C
```

Formula XYZ:

```
C          0.99597        -0.08208        -0.05184
C          2.49384         0.00263        -0.05550
C          2.97321         0.46442        -1.43103
C          2.97333         0.92259         1.07971
C          4.48717         0.94740         1.24047
H          0.50789        -0.97989        -0.41529
H          0.39238         0.80572         0.10324
H          2.88140        -1.00777         0.12560
H          2.67196         1.49834        -1.63394
H          2.55825        -0.16725        -2.22498
H          4.06327         0.40735        -1.51064
H          2.53498         0.58674         2.02855
H          2.61649         1.94754         0.91630
H          4.88529        -0.06350         1.37264
H          4.76080         1.53677         2.12162
H          4.97576         1.40331         0.37453
```

Energia:

```
C H A R G E S

IDX     CHARGE
1       -0.050226
2       -0.044120
3       -0.062423
4       -0.053312
5       -0.065034
6       0.026793
7       0.026793
8       0.029805
9       0.023242
10      0.023242
11      0.023242
12      0.026521
13      0.026521
14      0.022986
15      0.022986
16      0.022986

S E T T I N G  U P  C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP IMPROPER TORSION CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

E N E R G Y

     TOTAL BOND STRETCHING ENERGY =    2.159 kJ/mol
     TOTAL ANGLE BENDING ENERGY =   20.058 kJ/mol
     TOTAL TORSIONAL ENERGY =    3.252 kJ/mol
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol
     TOTAL VAN DER WAALS ENERGY =    5.662 kJ/mol
     TOTAL ELECTROSTATIC ENERGY =    0.373 kJ/mol

TOTAL ENERGY =   31.503 kJ/mol
```

Marcos André Lopes Mendes | nº mec: 90706 | Data: 21/10/2020

Neopentano

Formula Smiles:

```
C(-C)(-C)(-C)(-C)
```

Formula XYZ:

```
C          0.98290       -0.01082       -0.09792
C          0.47113        1.23120        0.64546
C          0.47112        0.01195       -1.54525
C          0.47111       -1.27564        0.60602
C          2.51824       -0.01081       -0.09793
H         -0.62419        1.25926        0.66225
H          0.82082        2.15208        0.16535
H          0.82082        1.24319        1.68391
H         -0.62419        0.01248       -1.57793
H          0.82081       -0.86426       -2.10270
H          0.82082        0.90530       -2.07483
H         -0.62422       -1.30422        0.62193
H          0.82079       -1.32029        1.64357
H          0.82079       -2.18095        0.09718
H          2.91417        0.88201       -0.59482
H          2.91417       -0.88753       -0.62268
H          2.91416       -0.02688        0.92372
```

Energia:

```
C H A R G E S

IDX     CHARGE
1       -0.040531
2       -0.060312
3       -0.060312
4       -0.060312
5       -0.060312
6       0.023482
7       0.023482
8       0.023482
9       0.023482
10      0.023482
11      0.023482
12      0.023482
13      0.023482
14      0.023482
15      0.023482
16      0.023482
17      0.023482

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP IMPROPER TORSION CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

E N E R G Y

     TOTAL BOND STRETCHING ENERGY =    0.246 kJ/mol
     TOTAL ANGLE BENDING ENERGY =    1.806 kJ/mol
     TOTAL TORSIONAL ENERGY =    0.000 kJ/mol
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mo
     TOTAL VAN DER WAALS ENERGY =    8.735 kJ/mol
     TOTAL ELECTROSTATIC ENERGY =    0.522 kJ/mol

TOTAL ENERGY =   11.309 kJ/mol
```

Marcos André Lopes Mendes | nº mec: 90706 | Data: 21/10/2020

Alinea d)

```
==> isopentano.xyz <==
16

C          0.99597       -0.08208       -0.05184

==> neopentano.xyz <==
17

C          0.98290       -0.01082       -0.09792

==> n-pentano.xyz <==
17

C          1.20735        0.32459        0.30375
```