

Lennard-Jones Second Virial Coefficient by James Pate Williams, Jr.

For the second virial coefficient and the Lennard-Jones Potential

Reference: **Introduction to Statistical**

Thermodynamics (c) 1960 by Terrell L. Hill

For the bisection root finding method

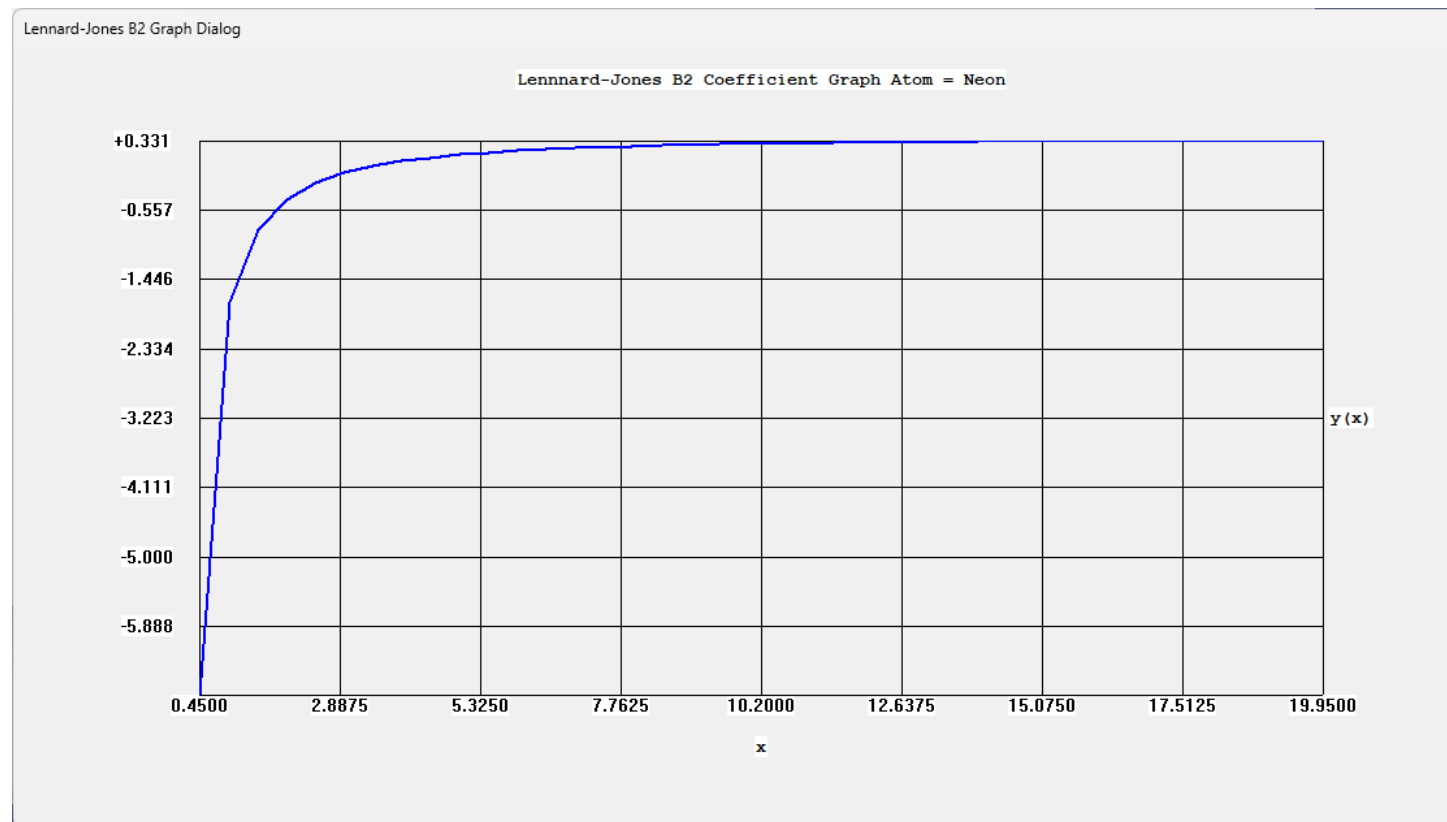
Reference: **Numerical Computation 2: Methods,**

Software, and Analysis (c) 1997 by Christoph

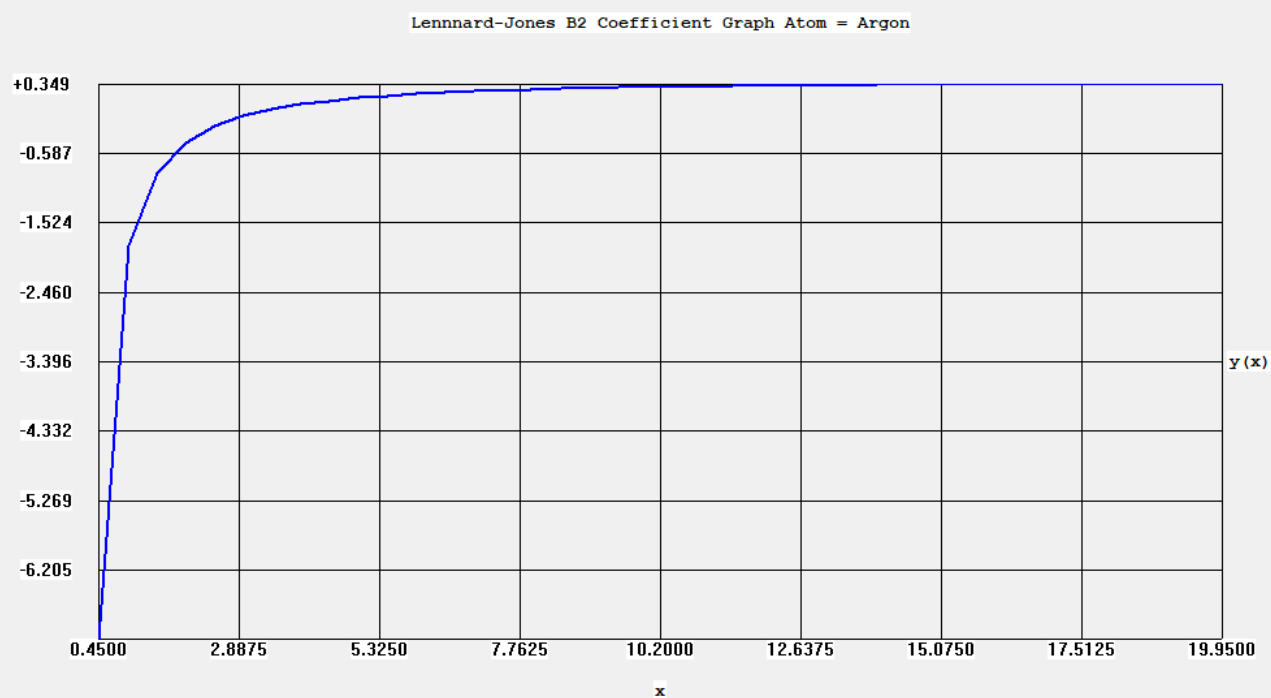
W. Ueberhuber

We graph the one-component classical gas second virial coefficient for neon, argon, xenon, nitrogen, oxygen, and methane. Each of these gases is spherically symmetric. The Boyle temperature appears to be a universal constant for these gases. We use Simpson's Rule to perform the integration of the formula illustrated below. The Lennard-Jones potential is utilized.

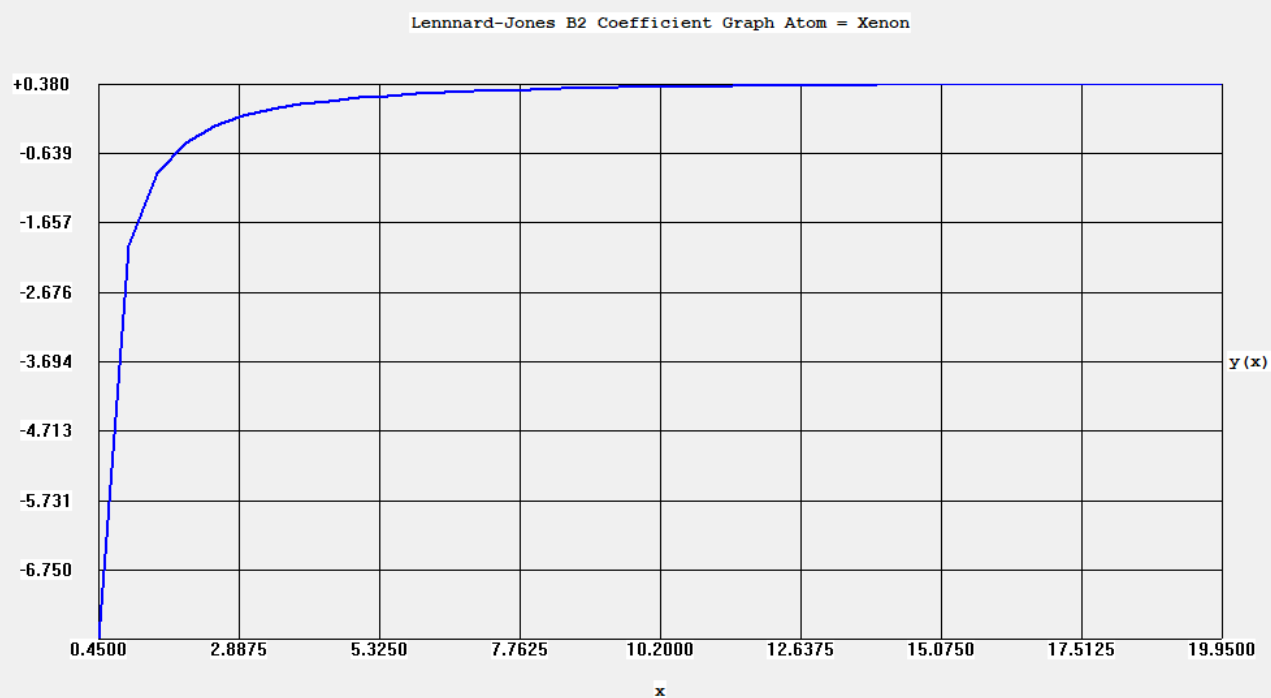
$$B_2(T) = -2\pi r^3 \int_0^{\infty} \left(e^{\frac{2\epsilon}{kT}y^{-6} - \frac{\epsilon}{kT}y^{-12}} - 1 \right) y^2 dy$$



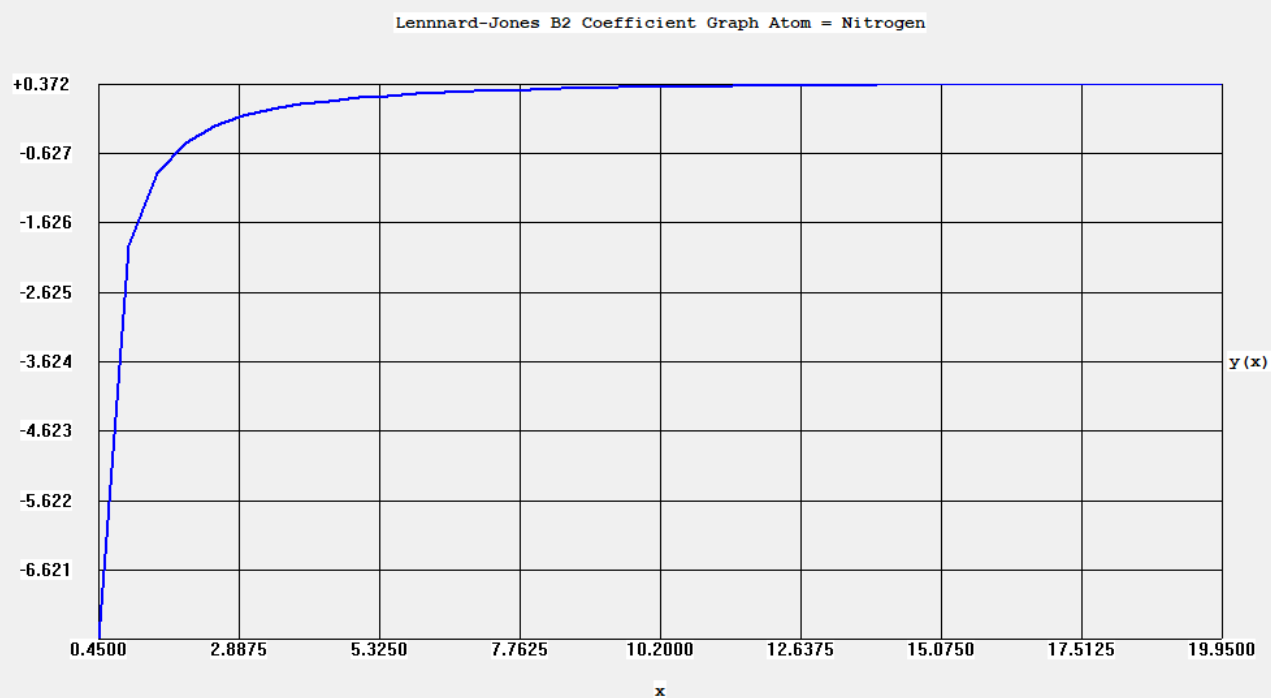
Lennard-Jones B2 Graph Dialog



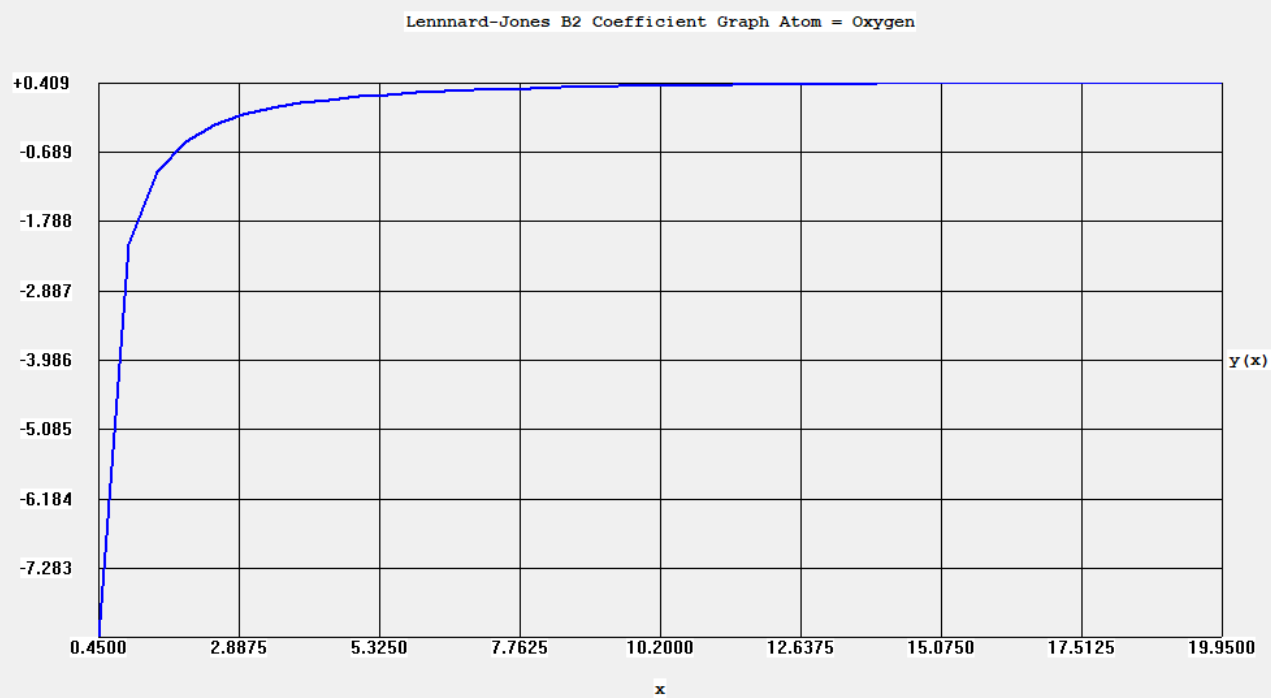
Lennard-Jones B2 Graph Dialog



Lennard-Jones B2 Graph Dialog

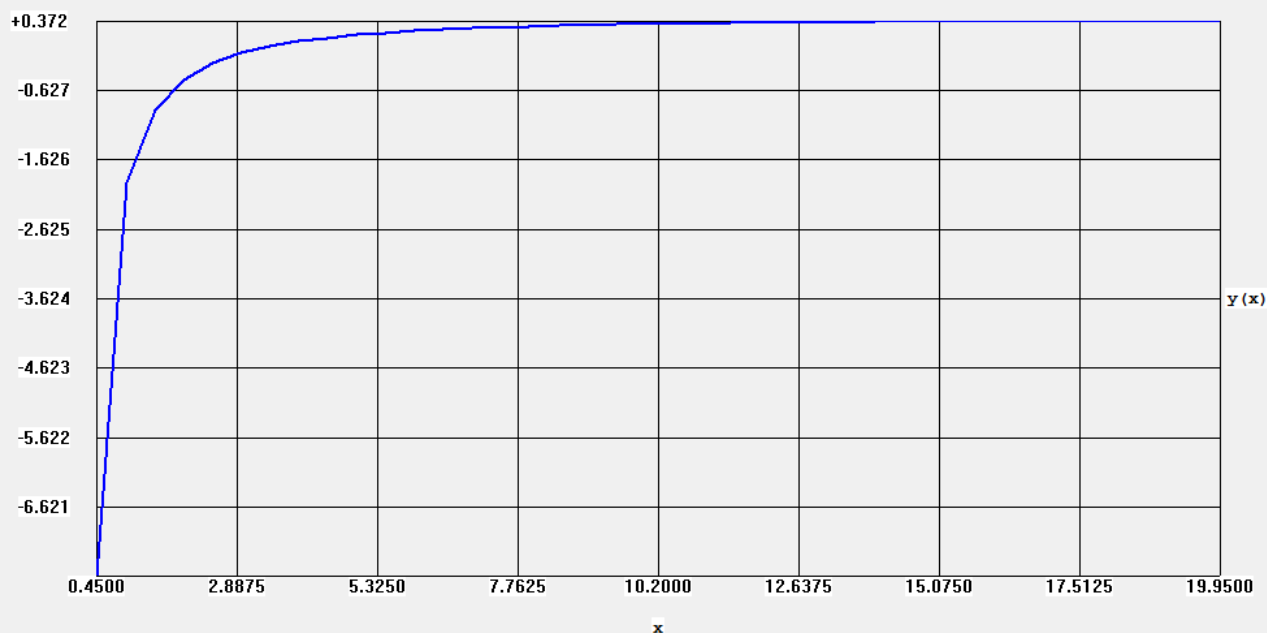


Lennard-Jones B2 Graph Dialog



Lennard-Jones B2 Graph Dialog

Lennard-Jones B2 Coefficient Graph Atom = Methane



Monatomic Atom = Neon

 $y = r/r^*$ Reduced B2

0.5	-6.7765706674
0.9	-1.7481827139
1.4	-0.8092598294
1.9	-0.4217033979
2.5	-0.2124739890
3.0	-0.0827211159
3.5	0.00489824498
4.0	0.06758123015
4.5	0.11433346057
5.0	0.15031888005
5.5	0.17870605897
6.0	0.20154418467
6.5	0.22021543505
7.0	0.23568474157
7.5	0.24864536698
8.0	0.25960765193
8.4	0.26895520096
8.9	0.27698162223
9.4	0.28391523196
9.9	0.28993607664

10.4	0.29518791693
10.9	0.29978682725
11.4	0.30382747312
11.9	0.30738776439
12.4	0.31053235278
12.9	0.31331529422
13.4	0.31578209897
13.9	0.31797132705
14.4	0.31991584196
14.9	0.32164380483
15.4	0.32317946920
15.9	0.32454382146
16.4	0.32575510061
16.9	0.32682922283
17.4	0.32778013063
17.9	0.32862008156
18.4	0.32935988828
18.9	0.33000911928
19.4	0.33057626748
19.9	0.33106889249

Boyle T = 3.41690095798

Monatomic Atom = Argon

y = r/r* Reduced B2

0.5	-7.1412291786
0.9	-1.8422553263
1.4	-0.8528074435
1.9	-0.4443959574
2.5	-0.2239075669
3.0	-0.0871724764
3.5	0.00516182767
4.0	0.07121788827
4.5	0.12048593378
5.0	0.15840778840
5.5	0.18832252851
6.0	0.21238961165
6.5	0.23206559299
7.0	0.24836732856
7.5	0.26202538673
8.0	0.27357757042
8.4	0.28342812657
8.9	0.29188646289
9.4	0.29919318166
9.9	0.30553801798
10.4	0.31107246852
10.9	0.31591885383
11.4	0.32017693356

11.9	0.32392881001
12.4	0.32724261392
12.9	0.33017531005
13.4	0.33277485766
13.9	0.33508189173
14.4	0.33713104422
14.9	0.33895199164
15.4	0.34057029265
15.9	0.34200806298
16.4	0.34328452306
16.9	0.34441644558
17.4	0.34541852331
17.9	0.34630367339
18.4	0.34708329034
18.9	0.34776745754
19.4	0.34836512492
19.9	0.34888425890

Boyle T = 3.41690095798

Monatomic Atom = Xenon

y = r/r* Reduced B2

0.5	-7.7682639358
0.9	-2.0040143306
1.4	-0.9276880971
1.9	-0.4834160903
2.5	-0.2435677435
3.0	-0.0948266451
3.5	0.00561506132
4.0	0.07747116627
4.5	0.13106518650
5.0	0.17231676494
5.5	0.20485816516
6.0	0.23103845560
6.5	0.25244208408
7.0	0.27017519155
7.5	0.28503249386
8.0	0.29759901562
8.4	0.30831449866
8.9	0.31751551817
9.4	0.32546380249
9.9	0.33236574639
10.4	0.33838614868
10.9	0.34365807026
11.4	0.34829003016
11.9	0.35237133967
12.4	0.35597611172
12.9	0.35916631288

13.4	0.36199411345
13.9	0.36450371637
14.4	0.36673279445
14.9	0.36871362993
15.4	0.37047402567
15.9	0.37203803924
16.4	0.37342657875
16.9	0.37465788958
17.4	0.37574795462
17.9	0.37671082520
18.4	0.37755889632
18.9	0.37830313674
19.4	0.37895328223
19.9	0.37951799870

Boyle T = 3.41690095798

Monatomic Atom = Nitrogen

y = r/r* Reduced B2

0.5	-7.6195890279
0.9	-1.9656599893
1.4	-0.9099333010
1.9	-0.4741641077
2.5	-0.2389061599
3.0	-0.0930117810
3.5	0.00550759603
4.0	0.07598846452
4.5	0.12855676188
5.0	0.16901883642
5.5	0.20093743473
6.0	0.22661666697
6.5	0.24761065663
7.0	0.26500437449
7.5	0.27957732651
8.0	0.29190334068
8.4	0.30241374271
8.9	0.31143866614
9.4	0.31923483019
9.9	0.32600467947
10.4	0.33190985875
10.9	0.33708088231
11.4	0.34162419227
11.9	0.34562739059
12.4	0.34916317179
12.9	0.35229231647
13.4	0.35506599645
13.9	0.35752756869
14.4	0.35971398498

14.9	0.36165690974
15.4	0.36338361369
15.9	0.36491769399
16.4	0.36627965858
16.9	0.36748740366
17.4	0.36855660621
17.9	0.36950104864
18.4	0.37033288873
18.9	0.37106288532
19.4	0.37170058784
19.9	0.37225449634

Boyle T = 3.41690095798

Monatomic Atom = Oxygen

$y = r/r^*$ Reduced B2

0.5	-8.3815479307
0.9	-2.1622259883
1.4	-1.0009266311
1.9	-0.5215805185
2.5	-0.2627967759
3.0	-0.1023129592
3.5	0.00605835563
4.0	0.08358731097
4.5	0.14141243807
5.0	0.18592072006
5.5	0.22103117820
6.0	0.24927833367
6.5	0.27237172230
7.0	0.29150481194
7.5	0.30753505916
8.0	0.32109367475
8.4	0.33265511698
8.9	0.34258253276
9.4	0.35115831321
9.9	0.35860514742
10.4	0.36510084463
10.9	0.37078897055
11.4	0.37578661149
11.9	0.38019012964
12.4	0.38407948896
12.9	0.38752154811
13.4	0.39057259609
13.9	0.39328032556
14.4	0.39568538348
14.9	0.39782260071
15.4	0.39972197506
15.9	0.40140946339

16.4	0.40290762444
16.9	0.40423614402
17.4	0.40541226683
17.9	0.40645115351
18.4	0.40736617761
18.9	0.40816917385
19.4	0.40887064662
19.9	0.40947994597

Boyle T = 3.41690095798

Monatomic Atom = Methane

y = r/r* Reduced B2

0.5	-7.6195890279
0.9	-1.9656599893
1.4	-0.9099333010
1.9	-0.4741641077
2.5	-0.2389061599
3.0	-0.0930117810
3.5	0.00550759603
4.0	0.07598846452
4.5	0.12855676188
5.0	0.16901883642
5.5	0.20093743473
6.0	0.22661666697
6.5	0.24761065663
7.0	0.26500437449
7.5	0.27957732651
8.0	0.29190334068
8.4	0.30241374271
8.9	0.31143866614
9.4	0.31923483019
9.9	0.32600467947
10.4	0.33190985875
10.9	0.33708088231
11.4	0.34162419227
11.9	0.34562739059
12.4	0.34916317179
12.9	0.35229231647
13.4	0.35506599645
13.9	0.35752756869
14.4	0.35971398498
14.9	0.36165690974
15.4	0.36338361369
15.9	0.36491769399
16.4	0.36627965858
16.9	0.36748740366
17.4	0.36855660621

17.9	0.36950104864
18.4	0.37033288873
18.9	0.37106288532
19.4	0.37170058784
19.9	0.37225449634

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