



ACD/Labs

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LogD Module Report

Date: July 25, 2022 12:06 PM

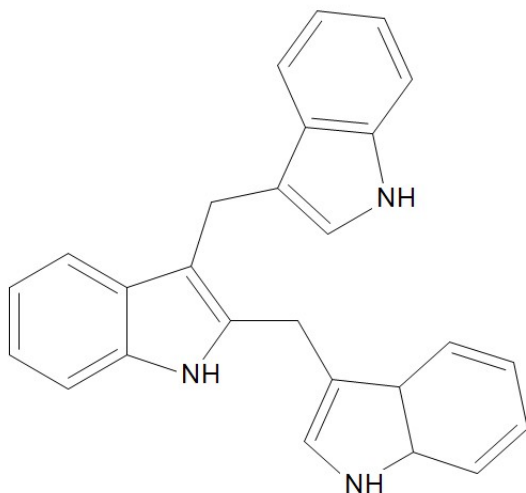
Software name and version: ACD/Percepta 14.52.0 (Build 3479)

Compound name: C:\Users\ZLYJ\Desktop\LTr1.cdx

pKa - Predicted using ACD/pKa GALAS

*LogP Predicted using ACD/LogP GALAS with the following trainable libraries:
LogP v. 1.3.trn*

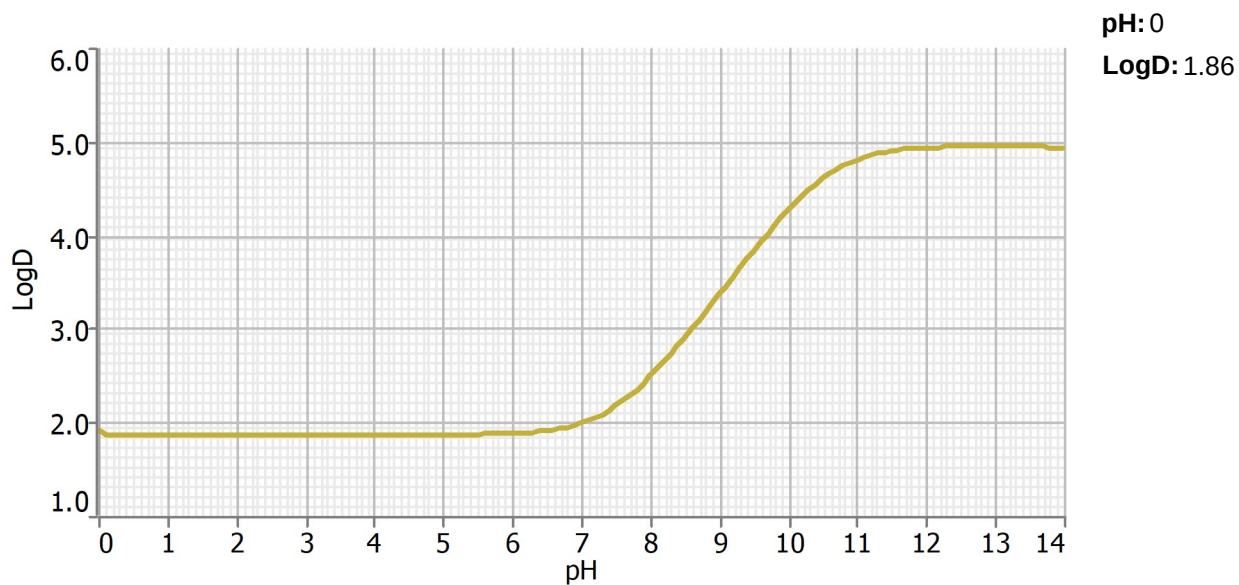
Structure:



LogD at:

pH = 1.7 (Stomach): 1.86
pH = 4.6 (Duodenum): 1.86
pH = 6.5 (Jejunum and Ileum): 1.9
pH = 7.4 (Blood): 2.11
pH = 8.0 (Colon): 2.48

LogD at given pH



pH	LogD
0	1.86
0.1	1.86
0.2	1.86
0.3	1.86
0.4	1.86
0.5	1.86
0.6	1.86
0.7	1.86
0.8	1.86
0.9	1.86
1	1.86
1.1	1.86
1.2	1.86
1.3	1.86
1.4	1.86
1.5	1.86
1.6	1.86
1.7	1.86
1.8	1.86
1.9	1.86
2	1.86
2.1	1.86
2.2	1.86
2.3	1.86
2.4	1.86
2.5	1.86
2.6	1.86
2.7	1.86

2.8	1.86
2.9	1.86
3	1.86
3.1	1.86
3.2	1.86
3.3	1.86
3.4	1.86
3.5	1.86
3.6	1.86
3.7	1.86
3.8	1.86
3.9	1.86
4	1.86
4.1	1.86
4.2	1.86
4.3	1.86
4.4	1.86
4.5	1.86
4.6	1.86
4.7	1.86
4.8	1.86
4.9	1.86
5	1.86
5.1	1.86
5.2	1.86
5.3	1.86
5.4	1.86
5.5	1.86
5.6	1.87
5.7	1.87
5.8	1.87
5.9	1.87
6	1.87
6.1	1.88
6.2	1.88
6.3	1.89
6.4	1.89
6.5	1.9
6.6	1.91
6.7	1.92
6.8	1.94
6.9	1.96
7	1.98
7.1	2.01
7.2	2.04
7.3	2.07
7.4	2.11
7.5	2.16
7.6	2.21
7.7	2.27
7.8	2.34
7.9	2.4

8	2.48
8.1	2.56
8.2	2.64
8.3	2.72
8.4	2.81
8.5	2.9
8.6	2.99
8.7	3.08
8.8	3.17
8.9	3.27
9	3.36
9.1	3.46
9.2	3.55
9.3	3.65
9.4	3.74
9.5	3.83
9.6	3.92
9.7	4.01
9.8	4.1
9.9	4.18
10	4.26
10.1	4.34
10.2	4.42
10.3	4.48
10.4	4.55
10.5	4.61
10.6	4.66
10.7	4.71
10.8	4.75
10.9	4.78
11	4.81
11.1	4.84
11.2	4.86
11.3	4.88
11.4	4.9
11.5	4.91
11.6	4.92
11.7	4.93
11.8	4.93
11.9	4.94
12	4.94
12.1	4.95
12.2	4.95
12.3	4.95
12.4	4.95
12.5	4.95
12.6	4.95
12.7	4.96
12.8	4.96
12.9	4.96
13	4.96
13.1	4.96

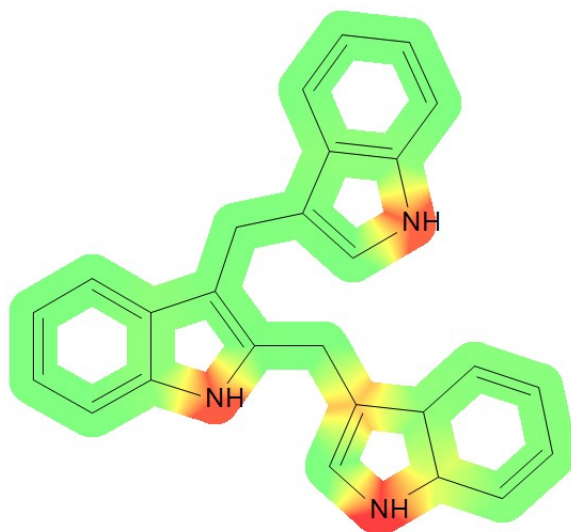
13.2	4.96
13.3	4.96
13.4	4.95
13.5	4.95
13.6	4.95
13.7	4.95
13.8	4.95
13.9	4.95
14	4.94

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Software name and version: ACD/Percepta 14.52.0 (Build 3479)

Compound name: C:\Users\ZLYJ\Desktop\LTr1.cdx

Structure:



LogP: 4.96

Reliability: Moderate (RI = 0.65)

Library used in calculation:

LogP v. 1.3 (Read-only)