

Aphyllidine

Inchi: InChI=1S/C15H22N2O/c18-15-12-9-11(13-5-2-4-8-17(13)15)10-16-7-3-1-6-14(12)16/h5,17-18,20-21,23-24,26-27,29-30,32-33,35-36,38-39,41-42,44-45,47-48,50-51,53-54,56-57,59-60,62-63,65-66,68-69,71-72,74-75,77-78,80-81,83-84,86-87,89-90,92-93,95-96,98-99,101-102,104-105,107-108,110-111,113-114,116-117,119-120,122-123,125-126,128-129,131-132,134-135,137-138,140-141,143-144,146-147,149-150,152-153,155-156,158-159,161-162,164-165,167-168,170-171,173-174,176-177,179-180,182-183,185-186,188-189,191-192,194-195,197-198,200-201,203-204,206-207,209-210,212-213,215-216,218-219,221-222,224-225,227-228,230-231,233-234,236-237,239-240,242-243,245-246,248-249,251-252,254-255,257-258,260-261,263-264,266-267,269-270,272-273,275-276,278-279,281-282,284-285,287-288,290-291,293-294,296-297,299-300,302-303,305-306,308-309,311-312,314-315,317-318,320-321,323-324,326-327,329-330,332-333,335-336,338-339,341-342,344-345,347-348,350-351,353-354,356-357,359-360,362-363,365-366,368-369,371-372,374-375,377-378,380-381,383-384,386-387,389-390,392-393,395-396,398-399,401-402,404-405,407-408,410-411,413-414,416-417,419-420,422-423,425-426,428-429,431-432,434-435,437-438,440-441,443-444,446-447,449-450,452-453,455-456,458-459,461-462,464-465,467-468,470-471,473-474,476-477,479-480,482-483,485-486,488-489,491-492,494-495,497-498,499,500,501,502,503,504,505,506,507,508,509,510,511,512,513,514,515,516,517,518,519,520,521,522,523,524,525,526,527,528,529,530,531,532,533,534,535,536,537,538,539,540,541,542,543,544,545,546,547,548,549,550,551,552,553,554,555,556,557,558,559,560,561,562,563,564,565,566,567,568,569,570,571,572,573,574,575,576,577,578,579,580,581,582,583,584,585,586,587,588,589,590,591,592,593,594,595,596,597,598,599,600,601,602,603,604,605,606,607,608,609,610,611,612,613,614,615,616,617,618,619,620,621,622,623,624,625,626,627,628,629,630,631,632,633,634,635,636,637,638,639,640,641,642,643,644,645,646,647,648,649,650,651,652,653,654,655,656,657,658,659,660,661,662,663,664,665,666,667,668,669,670,671,672,673,674,675,676,677,678,679,680,681,682,683,684,685,686,687,688,689,690,691,692,693,694,695,696,697,698,699,700,701,702,703,704,705,706,707,708,709,710,711,712,713,714,715,716,717,718,719,720,721,722,723,724,725,726,727,728,729,730,731,732,733,734,735,736,737,738,739,740,741,742,743,744,745,746,747,748,749,750,751,752,753,754,755,756,757,758,759,760,761,762,763,764,765,766,767,768,769,770,771,772,773,774,775,776,777,778,779,780,781,782,783,784,785,786,787,788,789,790,791,792,793,794,795,796,797,798,799,800,801,802,803,804,805,806,807,808,809,810,811,812,813,814,815,816,817,818,819,820,821,822,823,824,825,826,827,828,829,830,831,832,833,834,835,836,837,838,839,840,841,842,843,844,845,846,847,848,849,850,851,852,853,854,855,856,857,858,859,860,861,862,863,864,865,866,867,868,869,870,871,872,873,874,875,876,877,878,879,880,881,882,883,884,885,886,887,888,889,890,891,892,893,894,895,896,897,898,899,900,901,902,903,904,905,906,907,908,909,910,911,912,913,914,915,916,917,918,919,920,921,922,923,924,925,926,927,928,929,930,931,932,933,934,935,936,937,938,939,940,941,942,943,944,945,946,947,948,949,950,951,952,953,954,955,956,957,958,959,960,961,962,963,964,965,966,967,968,969,970,971,972,973,974,975,976,977,978,979,980,981,982,983,984,985,986,987,988,989,990,991,992,993,994,995,996,997,998,999,1000

InchiKey: UAAWNTMXVSONPU-ORHYLEIMSA-N

Formula: C15H22N2O

SMILES: O=C1C2CC(CN3CCCCC23)C2=CCCCN12

Mol. weight [g/mol]: 246.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	1.997		Crippen Method
mcvol	196.000	ml/mol	McGowan Method
rinpol	2120.00		NIST Webbook
rinpol	2127.00		NIST Webbook
rinpol	2120.00		NIST Webbook
rinpol	2120.00		NIST Webbook
rinpol	2127.00		NIST Webbook
rinpol	2145.00		NIST Webbook
rinpol	2125.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R205419&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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