

Ipanguline D12

Inchi: InChI=1S/C13H23NO5/c1-8(16)13(2,18)12(17)19-10-4-6-14-5-3-9(7-15)11(10)14/h8-11,13,17,19,21,23,25,27,29,31,33,35,37,39,41,43,45,47,49,51,53,55,57,59,61,63,65,67,69,71,73,75,77,79,81,83,85,87,89,91,93,95,97,99,101,103,105,107,109,111,113,115,117,119,121,123,125,127,129,131,133,135,137,139,141,143,145,147,149,151,153,155,157,159,161,163,165,167,169,171,173,175,177,179,181,183,185,187,189,191,193,195,197,199,201,203,205,207,209,211,213,215,217,219,221,223,225,227,229,231,233,235,237,239,241,243,245,247,249,251,253,255,257,259,261,263,265,267,269,271,273,275,277,279,281,283,285,287,289,291,293,295,297,299,301,303,305,307,309,311,313,315,317,319,321,323,325,327,329,331,333,335,337,339,341,343,345,347,349,351,353,355,357,359,361,363,365,367,369,371,373,375,377,379,381,383,385,387,389,391,393,395,397,399,401,403,405,407,409,411,413,415,417,419,421,423,425,427,429,431,433,435,437,439,441,443,445,447,449,451,453,455,457,459,461,463,465,467,469,471,473,475,477,479,481,483,485,487,489,491,493,495,497,499,501,503,505,507,509,511,513,515,517,519,521,523,525,527,529,531,533,535,537,539,541,543,545,547,549,551,553,555,557,559,561,563,565,567,569,571,573,575,577,579,581,583,585,587,589,591,593,595,597,599,601,603,605,607,609,611,613,615,617,619,621,623,625,627,629,631,633,635,637,639,641,643,645,647,649,651,653,655,657,659,661,663,665,667,669,671,673,675,677,679,681,683,685,687,689,691,693,695,697,699,701,703,705,707,709,711,713,715,717,719,721,723,725,727,729,731,733,735,737,739,741,743,745,747,749,751,753,755,757,759,761,763,765,767,769,771,773,775,777,779,781,783,785,787,789,791,793,795,797,799,801,803,805,807,809,811,813,815,817,819,821,823,825,827,829,831,833,835,837,839,841,843,845,847,849,851,853,855,857,859,861,863,865,867,869,871,873,875,877,879,881,883,885,887,889,891,893,895,897,899,901,903,905,907,909,911,913,915,917,919,921,923,925,927,929,931,933,935,937,939,941,943,945,947,949,951,953,955,957,959,961,963,965,967,969,971,973,975,977,979,981,983,985,987,989,991,993,995,997,999

InchiKey: JUKASHKBUGPLHM-LFEBVRLFSA-N

Formula: C13H23NO5

SMILES: CC(O)C(C)(O)C(=O)OC1CCN2CCCC(CO)C12

Mol. weight [g/mol]: 273.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.48		Crippen Method
logp	-0.883		Crippen Method
mcvol	207.340	ml/mol	McGowan Method
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook

Sources

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=R394960&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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<https://www.chemeo.com/cid/13-221-1/lpanguline-D12.pdf>

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