

DL-Alanine, N-methyl-N-(3-chloro-2-methylpropoxycarbonyl)-, hexyl ester

InChI: InChI=1S/C15H28ClNO4/c1-5-6-7-8-9-20-14(18)13(3)17(4)15(19)21-11-12(2)10-16/h12-14,20-21,23-24,26-27,29-30,32-33,35-36,38-39,41-42,44-45,47-48,50-51,53-54,56-57,59-60,62-63,65-66,68-69,71-72,74-75,77-78,80-81,83-84,86-87,89-90,92-93,95-96,98-99,101-102,104-105,107-108,110-111,113-114,116-117,119-120,122-123,125-126,128-129,131-132,134-135,137-138,140-141,143-144,146-147,149-150,152-153,155-156,158-159,161-162,164-165,167-168,170-171,173-174,176-177,179-180,182-183,185-186,188-189,191-192,194-195,197-198,200-201,203-204,206-207,209-210,212-213,215-216,218-219,221-222,224-225,227-228,230-231,233-234,236-237,239-240,242-243,245-246,248-249,251-252,254-255,257-258,260-261,263-264,266-267,269-270,272-273,275-276,278-279,281-282,284-285,287-288,290-291,293-294,296-297,299-300,302-303,305-306,308-309,311-312,314-315,317-318,320-321,323-324,326-327,329-330,332-333,335-336,338-339,341-342,344-345,347-348,350-351,353-354,356-357,359-360,362-363,365-366,368-369,371-372,374-375,377-378,380-381,383-384,386-387,389-390,392-393,395-396,398-399,401-402,404-405,407-408,410-411,413-414,416-417,419-420,422-423,425-426,428-429,431-432,434-435,437-438,440-441,443-444,446-447,449-450,452-453,455-456,458-459,461-462,464-465,467-468,470-471,473-474,476-477,479-480,482-483,485-486,488-489,491-492,494-495,497-498,499,500,501,502,503,504,505,506,507,508,509,510,511,512,513,514,515,516,517,518,519,520,521,522,523,524,525,526,527,528,529,530,531,532,533,534,535,536,537,538,539,540,541,542,543,544,545,546,547,548,549,550,551,552,553,554,555,556,557,558,559,560,561,562,563,564,565,566,567,568,569,570,571,572,573,574,575,576,577,578,579,580,581,582,583,584,585,586,587,588,589,590,591,592,593,594,595,596,597,598,599,600,601,602,603,604,605,606,607,608,609,610,611,612,613,614,615,616,617,618,619,620,621,622,623,624,625,626,627,628,629,630,631,632,633,634,635,636,637,638,639,640,641,642,643,644,645,646,647,648,649,650,651,652,653,654,655,656,657,658,659,660,661,662,663,664,665,666,667,668,669,670,671,672,673,674,675,676,677,678,679,680,681,682,683,684,685,686,687,688,689,690,691,692,693,694,695,696,697,698,699,700,701,702,703,704,705,706,707,708,709,710,711,712,713,714,715,716,717,718,719,720,721,722,723,724,725,726,727,728,729,730,731,732,733,734,735,736,737,738,739,740,741,742,743,744,745,746,747,748,749,750,751,752,753,754,755,756,757,758,759,760,761,762,763,764,765,766,767,768,769,770,771,772,773,774,775,776,777,778,779,780,781,782,783,784,785,786,787,788,789,790,791,792,793,794,795,796,797,798,799,800,801,802,803,804,805,806,807,808,809,810,811,812,813,814,815,816,817,818,819,820,821,822,823,824,825,826,827,828,829,830,831,832,833,834,835,836,837,838,839,840,841,842,843,844,845,846,847,848,849,850,851,852,853,854,855,856,857,858,859,860,861,862,863,864,865,866,867,868,869,870,871,872,873,874,875,876,877,878,879,880,881,882,883,884,885,886,887,888,889,890,891,892,893,894,895,896,897,898,899,900,901,902,903,904,905,906,907,908,909,910,911,912,913,914,915,916,917,918,919,920,921,922,923,924,925,926,927,928,929,930,931,932,933,934,935,936,937,938,939,940,941,942,943,944,945,946,947,948,949,950,951,952,953,954,955,956,957,958,959,960,961,962,963,964,965,966,967,968,969,970,971,972,973,974,975,976,977,978,979,980,981,982,983,984,985,986,987,988,989,990,991,992,993,994,995,996,997,998,999,1000

InChIKey:

ZOUPGIACDVMQQM-UHFFFAOYSA-N

Formula:

C15H28ClNO4

SMILES:

CCCCCOC(=O)C(C)N(C)C(=O)OCC(C)CCI

Mol. weight [g/mol]:

321.84

Physical Properties

Property code	Value	Unit	Source
gf	-298.45	kJ/mol	Joback Method
hf	-801.30	kJ/mol	Joback Method
hfus	40.35	kJ/mol	Joback Method
hvap	72.95	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.442		Crippen Method
mvol	259.310	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	1942.00		NIST Webbook
rinpol	1942.00		NIST Webbook
tb	744.17	K	Joback Method
tc	928.55	K	Joback Method
tf	435.52	K	Joback Method
vc	0.979	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.23	J/molxK	744.17	Joback Method
cpg	766.05	J/molxK	774.90	Joback Method
cpg	780.98	J/molxK	805.63	Joback Method
cpg	795.03	J/molxK	836.36	Joback Method
cpg	808.21	J/molxK	867.09	Joback Method
cpg	820.54	J/molxK	897.82	Joback Method
cpg	832.04	J/molxK	928.55	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392767&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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