

I-Norvaline, N-allyloxycarbonyl-, octyl ester

Inchi:	InChI=1S/C17H31NO4/c1-4-7-8-9-10-11-14-21-16(19)15(12-5-2)18-17(20)22-13-6-3/h6,17-19,20-21,23-24,26-27,29-30,32-33,35-36,38-39,41-42,44-45,47-48,49-50,52-53,55-56,58-59,61-62,64-65,67-68,69-70,72-73,75-76,78-79,81-82,84-85,87-88,89-90,92-93,95-96,98-99,100-101,103-104,106-107,109-110,112-113,115-116,118-119,120-121,123-124,126-127,129-130,132-133,135-136,138-139,140-141,143-144,146-147,149-150,152-153,155-156,158-159,161-162,164-165,167-168,169-170,172-173,175-176,178-179,180-181,183-184,186-187,189-190,192-193,195-196,198-199,199-200,201-202,203-204,205-206,207-208,209-209,210-211,212-213,214-215,216-217,218-219,219-220,221-222,223-224,225-226,227-228,229-229,230-231,232-233,234-235,236-237,238-239,239-240,241-242,243-244,245-246,247-248,249-249,250-251,252-253,254-255,256-257,258-259,259-260,261-262,263-264,265-266,267-268,269-269,270-271,272-273,274-275,276-277,278-279,279-280,281-282,283-284,285-286,287-288,289-289,290-291,292-293,294-295,296-297,298-299,299-300,301-302,303-304,305-306,307-308,309-309,310-311,312-313,314-315,316-317,318-319,320-321,322-323,324-325,326-327,328-329,330-331,332-333,334-335,336-337,338-339,340-341,342-343,344-345,346-347,348-349,350-351,352-353,354-355,356-357,358-359,360-361,362-363,364-365,366-367,368-369,370-371,372-373,374-375,376-377,378-379,380-381,382-383,384-385,386-387,388-389,390-391,392-393,394-395,396-397,398-399,399-400,401-402,403-404,405-406,407-408,409-409,410-411,412-413,414-415,416-417,418-419,420-421,422-423,424-425,426-427,428-429,430-431,432-433,434-435,436-437,438-439,440-441,442-443,444-445,446-447,448-449,450-451,452-453,454-455,456-457,458-459,460-461,462-463,464-465,466-467,468-469,470-471,472-473,474-475,476-477,478-479,480-481,482-483,484-485,486-487,488-489,490-491,492-493,494-495,496-497,498-499,499-500,501-502,503-504,505-506,507-508,509-509,510-511,512-513,514-515,516-517,518-519,520-521,522-523,524-525,526-527,528-529,530-531,532-533,534-535,536-537,538-539,540-541,542-543,544-545,546-547,548-549,550-551,552-553,554-555,556-557,558-559,560-561,562-563,564-565,566-567,568-569,570-571,572-573,574-575,576-577,578-579,580-581,582-583,584-585,586-587,588-589,590-591,592-593,594-595,596-597,598-599,599-600,601-602,603-604,605-606,607-608,609-609,610-611,612-613,614-615,616-617,618-619,620-621,622-623,624-625,626-627,628-629,630-631,632-633,634-635,636-637,638-639,640-641,642-643,644-645,646-647,648-649,650-651,652-653,654-655,656-657,658-659,660-661,662-663,664-665,666-667,668-669,670-671,672-673,674-675,676-677,678-679,680-681,682-683,684-685,686-687,688-689,690-691,692-693,694-695,696-697,698-699,699-700,701-702,703-704,705-706,707-708,709-709,710-711,712-713,714-715,716-717,718-719,720-721,722-723,724-725,726-727,728-729,730-731,732-733,734-735,736-737,738-739,740-741,742-743,744-745,746-747,748-749,750-751,752-753,754-755,756-757,758-759,760-761,762-763,764-765,766-767,768-769,770-771,772-773,774-775,776-777,778-779,780-781,782-783,784-785,786-787,788-789,790-791,792-793,794-795,796-797,798-799,799-800,801-802,803-804,805-806,807-808,809-809,810-811,812-813,814-815,816-817,818-819,820-821,822-823,824-825,826-827,828-829,830-831,832-833,834-835,836-837,838-839,840-841,842-843,844-845,846-847,848-849,850-851,852-853,854-855,856-857,858-859,860-861,862-863,864-865,866-867,868-869,870-871,872-873,874-875,876-877,878-879,880-881,882-883,884-885,886-887,888-889,890-891,892-893,894-895,896-897,898-899,899-900,901-902,903-904,905-906,907-908,909-909,910-911,912-913,914-915,916-917,918-919,920-921,922-923,924-925,926-927,928-929,930-931,932-933,934-935,936-937,938-939,940-941,942-943,944-945,946-947,948-949,950-951,952-953,954-955,956-957,958-959,960-961,962-963,964-965,966-967,968-969,970-971,972-973,974-975,976-977,978-979,980-981,982-983,984-985,986-987,988-989,990-991,992-993,994-995,996-997,998-999,999-1000		
InchiKey:	WPOZNBKUDJCGDA-UHFFFAOYSA-N		
Formula:	C17H31NO4		
SMILES:	C=CCOC(O)=NC(CCC)C(=O)OCCCCCC		
Mol. weight [g/mol]:	313.43		

Physical Properties

Property code	Value	Unit	Source
hf	-730.88	kJ/mol	Joback Method
hvap	84.02	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.175		Crippen Method
mcvol	270.950	ml/mol	McGowan Method
pc	1294.86	kPa	Joback Method
rinpol	1919.00		NIST Webbook
rinpol	1919.00		NIST Webbook
tb	852.05	K	Joback Method
tc	1045.38	K	Joback Method

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320748&Units=SI>

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

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf: Enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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