

# Pipecolic acid, N-propargyloxycarbonyl-, hexyl ester

**Inchi:** InChI=1S/C16H25NO4/c1-3-5-6-9-13-20-15(18)14-10-7-8-11-17(14)16(19)21-12-4-2/h2,3-4,11-15,17,19-21,23-24,27-28,30-31,33-34,36-37,39-40,42-43,45-46,48-49,51-52,54-55,57-58,60-61,63-64,66-67,69-70,72-73,75-76,78-79,81-82,84-85,87-88,90-91,93-94,96-97,99-100,102-103,105-106,108-109,111-112,114-115,117-118,120-121,123-124,126-127,129-130,132-133,135-136,138-139,141-142,144-145,147-148,150-151,153-154,156-157,159-160,162-163,165-166,168-169,171-172,174-175,177-178,180-181,183-184,186-187,189-190,192-193,195-196,198-199,201-202,204-205,207-208,210-211,213-214,216-217,219-220,222-223,225-226,228-229,231-232,234-235,237-238,240-241,243-244,246-247,249-250,252-253,255-256,258-259,261-262,264-265,267-268,270-271,273-274,276-277,279-280,282-283,285-286,288-289,291-292,294-295,297-298,300-301,303-304,306-307,309-310,312-313,315-316,318-319,321-322,324-325,327-328,330-331,333-334,336-337,339-340,342-343,345-346,348-349,351-352,354-355,357-358,360-361,363-364,366-367,369-370,372-373,375-376,378-379,381-382,384-385,387-388,390-391,393-394,396-397,399-400,402-403,405-406,408-409,411-412,414-415,417-418,420-421,423-424,426-427,429-430,432-433,435-436,438-439,441-442,444-445,447-448,450-451,453-454,456-457,459-460,462-463,465-466,468-469,471-472,474-475,477-478,480-481,483-484,486-487,489-490,492-493,495-496,498-499,500,502-503,505-506,508-509,511-512,514-515,517-518,520-521,523-524,526-527,529-530,532-533,535-536,538-539,541-542,544-545,547-548,550-551,553-554,556-557,559-560,562-563,565-566,568-569,571-572,574-575,577-578,580-581,583-584,586-587,589-590,592-593,595-596,598-599,600,602-603,605-606,608-609,611-612,614-615,617-618,620-621,623-624,626-627,629-630,632-633,635-636,638-639,641-642,644-645,647-648,650-651,653-654,656-657,659-660,662-663,665-666,668-669,671-672,674-675,677-678,680-681,683-684,686-687,689-690,692-693,695-696,698-699,700,702-703,705-706,708-709,711-712,714-715,717-718,720-721,723-724,726-727,729-730,732-733,735-736,738-739,741-742,744-745,747-748,750-751,753-754,756-757,759-760,762-763,765-766,768-769,771-772,774-775,777-778,780-781,783-784,786-787,789-790,792-793,795-796,798-799,800,802-803,805-806,808-809,811-812,814-815,817-818,820-821,823-824,826-827,829-830,832-833,835-836,838-839,841-842,844-845,847-848,850-851,853-854,856-857,859-860,862-863,865-866,868-869,871-872,874-875,877-878,880-881,883-884,886-887,889-890,892-893,895-896,898-899,900,902-903,905-906,908-909,911-912,914-915,917-918,920-921,923-924,926-927,929-930,932-933,935-936,938-939,941-942,944-945,947-948,950-951,953-954,956-957,959-960,962-963,965-966,968-969,971-972,974-975,977-978,980-981,983-984,986-987,989-990,992-993,995-996,998-999,1000

**InchiKey:** HICHRLQMQQPDRA-UHFFFAOYSA-N

**Formula:** C16H25NO4

**SMILES:** C#CCOC(=O)N1CCCCC1C(=O)OCCCCC

**Mol. weight [g/mol]:** 295.37

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.734		Crippen Method
mcvol	241.700	ml/mol	McGowan Method
rmpol	2085.00		NIST Webbook
rmpol	2085.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393094&Units=SI>

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

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

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

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rmpol:** Non-polar retention indices

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