# 1-Aminocyclopentanecarboxylic acid, N-(but-2-yn-1-yloxycarbonyl)-, butyl ester

**Inchi:** InChI=1S/C15H23NO4/c1-3-5-11-19-13(17)15(9-7-8-10-15)16-14(18)20-12-6-4-2/h3,5,7-

**InchiKey:** NTFGVSITRJNDHM-UHFFFAOYSA-N

**Formula:** C15H23NO4

**SMILES:** CC#CCOC(O)=NC1(C(=O)OCCCC)CCCC1

**Mol. weight [g/mol]:** 281.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -461.73 | kJ/mol | Joback Method |
| hvap | 81.88 | kJ/mol | Joback Method |
| log10ws | -3.33 | | Crippen Method |
| logp | 2.596 | | Crippen Method |
| mcvol | 227.610 | ml/mol | McGowan Method |
| pc | 1971.80 | kPa | Joback Method |
| rinpol | 2013.00 | | NIST Webbook |
| rinpol | 2013.00 | | NIST Webbook |
| tb | 834.57 | K | Joback Method |
| tc | 1049.75 | K | 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=U392581&Units=SI

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

## 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 |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |

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