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

Inchi: InChI=1S/C15H19NO4/c1-3-5-11-19-13(17)15(9-7-8-10-15)16-14(18)20-12-6-4-2/h7-12H
InchiKey: GIXKYLSBYLERFJ-UHFFFAOYSA-N
Formula: C15H19NO4
SMILES: CC#CCOC(=O)C1(N=C(O)OCC#CC)CCCC1
Mol. weight [g/mol]: 277.32

Physical Properties

Property code	Value	Unit	Source
hf	-189.43	kJ/mol	Joback Method
hvap	84.03	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	1.820		Crippen Method
mcvol	219.010	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinpol	2102.00		NIST Webbook
rinpol	2102.00		NIST Webbook
tb	843.57	K	Joback Method
tc	1076.12	K	Joback Method

Sources

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=U392589&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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