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

Inchi: InChI=1S/C15H23NO4/c1-4-5-10-19-14(18)16-15(8-6-7-9-15)13(17)20-11-12(2)3/h12H,6

InchiKey: PTHGEARXTHKMAE-UHFFFAOYSA-N

Formula: C15H23NO4

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

Mol. weight [g/mol]: 281.35

Physical Properties

Property code	Value	Unit	Source
hf	-467.01	kJ/mol	Joback Method
hvap	81.49	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.452		Crippen Method
mcvol	227.610	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	1974.00		NIST Webbook
rinpol	1974.00		NIST Webbook
tb	834.13	K	Joback Method
tc	1052.12	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=U392580&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