1-Aminocyclopentanecarboxylic acid, N-(but-3-en-1-yloxycarbonyl)-, isobutyl ester

Inchi: InChI=1S/C15H25NO4/c1-4-5-10-19-14(18)16-15(8-6-7-9-15)13(17)20-11-12(2)3/h4,12H

InchiKey: KHUSIHHOTJFEEQ-UHFFFAOYSA-N

Formula: C15H25NO4

SMILES: C=CCCOC(O)=NC1(C(=O)OCC(C)C)CCCC1

Mol. weight [g/mol]: 283.36

Physical Properties

Property code	Value	Unit	Source
hf	-613.88	kJ/mol	Joback Method
hvap	78.67	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	3.005		Crippen Method
mcvol	231.910	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	1854.00		NIST Webbook
rinpol	1854.00		NIST Webbook
tb	821.81	K	Joback Method
tc	1027.35	K	Joback Method

Sources

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

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=U392592&Units=SI

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