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

Inchi: InChI=1S/C14H21NO4/c1-3-5-11-19-13(17)15-14(8-6-7-9-14)12(16)18-10-4-2/h4,6-11H2

InchiKey: CGVYONSCVSFQJI-UHFFFAOYSA-N

Formula: C14H21NO4

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

Mol. weight [g/mol]: 267.32

Physical Properties

Property code	Value	Unit	Source
gf	-77.59	kJ/mol	Joback Method
hf	-420.40	kJ/mol	Joback Method
hfus	33.45	kJ/mol	Joback Method
hvap	72.76	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.002		Crippen Method
mcvol	213.520	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	1929.00		NIST Webbook
rinpol	1929.00		NIST Webbook
tb	746.99	K	Joback Method
tc	966.88	K	Joback Method
tf	585.42	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.23	J/mol×K	746.99	Joback Method
cpg	636.69	J/mol×K	783.64	Joback Method
cpg	652.44	J/mol×K	820.29	Joback Method
cpg	667.60	J/mol×K	856.93	Joback Method
cpg	682.26	J/mol×K	893.58	Joback Method
cpg	696.54	J/mol×K	930.23	Joback Method
cpg	710.54	J/mol×K	966.88	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=U392579&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume