1-Aminocyclopentanecarboxylic acid, N-(but-3-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/h1H,4-11H

InchiKey: ALHRDTOJBJHDRB-UHFFFAOYSA-N

Formula: C14H21NO4

SMILES: C#CCCOC(=O)NC1(C(=O)OCCC)CCCC1

Mol. weight [g/mol]: 267.32

Physical Properties

Property code	Value	Unit	Source
gf	-57.32	kJ/mol	Joback Method
hf	-400.80	kJ/mol	Joback Method
hfus	33.30	kJ/mol	Joback Method
hvap	70.47	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.002		Crippen Method
mcvol	213.520	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	1835.00		NIST Webbook
rinpol	1835.00		NIST Webbook
tb	728.11	K	Joback Method
tc	939.66	K	Joback Method
tf	526.29	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.88	J/mol×K	728.11	Joback Method
cpg	632.77	J/mol×K	763.37	Joback Method
cpg	647.96	J/mol×K	798.63	Joback Method
cpg	662.56	J/mol×K	833.89	Joback Method
cpg	676.67	J/mol×K	869.15	Joback Method
cpg	690.39	J/mol×K	904.40	Joback Method
cpg	703.83	J/mol×K	939.66	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=U392568&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