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

Inchi: InChI=1S/C14H23NO4/c1-3-5-11-19-13(17)15-14(8-6-7-9-14)12(16)18-10-4-2/h3H,1,4-1

InchiKey: JDBJGYROYZDNKZ-UHFFFAOYSA-N

Formula: C14H23NO4

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

Mol. weight [g/mol]: 269.34

Physical Properties

Property code	Value	Unit	Source
gf	-192.55	kJ/mol	Joback Method
hf	-567.27	kJ/mol	Joback Method
hfus	29.05	kJ/mol	Joback Method
hvap	69.94	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.555		Crippen Method
mcvol	217.820	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinpol	1808.00		NIST Webbook
rinpol	1808.00		NIST Webbook
tb	734.67	K	Joback Method
tc	938.91	K	Joback Method
tf	477.56	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.47	J/mol×K	734.67	Joback Method
cpg	658.76	J/mol×K	768.71	Joback Method
cpg	674.36	J/mol×K	802.75	Joback Method
cpg	689.34	J/mol×K	836.79	Joback Method
cpg	703.81	J/mol×K	870.83	Joback Method
cpg	717.85	J/mol×K	904.87	Joback Method
cpg	731.57	J/mol×K	938.91	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=U392591&Units=SI

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