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

Inchi: InChI=1S/C13H21NO4/c1-3-5-10-18-12(16)14-13(8-6-7-9-13)11(15)17-4-2/h3H,1,4-10H2

InchiKey: JUXHCVATXCVWDL-UHFFFAOYSA-N

Formula: C13H21NO4

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

Mol. weight [g/mol]: 255.31

Physical Properties

Property code	Value	Unit	Source
gf	-200.97	kJ/mol	Joback Method
hf	-546.63	kJ/mol	Joback Method
hfus	26.46	kJ/mol	Joback Method
hvap	67.72	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.165		Crippen Method
mcvol	203.730	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
tb	711.79	K	Joback Method
tc	918.31	K	Joback Method
tf	466.29	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.63	J/mol×K	711.79	Joback Method
cpg	603.44	J/mol×K	746.21	Joback Method
cpg	618.54	J/mol×K	780.63	Joback Method
cpg	633.01	J/mol×K	815.05	Joback Method
cpg	646.96	J/mol×K	849.47	Joback Method
cpg	660.47	J/mol×K	883.89	Joback Method
cpg	673.63	J/mol×K	918.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392590&Units=SI
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

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