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

Inchi: InChI=1S/C17H29NO4/c1-3-5-7-10-14-21-15(19)17(11-8-9-12-17)18-16(20)22-13-6-4-2/h

InchiKey: GVVKLZNFNBTIOQ-UHFFFAOYSA-N

Formula: C17H29NO4

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

Mol. weight [g/mol]: 311.42

Physical Properties

Property code	Value	Unit	Source
gf	-167.29	kJ/mol	Joback Method
hf	-629.19	kJ/mol	Joback Method
hfus	36.82	kJ/mol	Joback Method
hvap	76.62	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	3.725		Crippen Method
mcvol	260.090	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
rinpol	2085.00		NIST Webbook
rinpol	2085.00		NIST Webbook
tb	803.31	K	Joback Method
tc	1003.80	K	Joback Method
tf	511.37	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.02	J/mol×K	803.31	Joback Method
cpg	831.71	J/mol×K	836.73	Joback Method
cpg	848.74	J/mol×K	870.14	Joback Method
cpg	865.20	J/mol×K	903.56	Joback Method
cpg	881.19	J/mol×K	936.97	Joback Method
cpg	896.81	J/mol×K	970.39	Joback Method
cpg	912.15	J/mol×K	1003.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392594&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