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

Inchi: InChI=1S/C16H27NO4/c1-3-5-9-13-20-14(18)16(10-7-8-11-16)17-15(19)21-12-6-4-2/h4H

InchiKey: FQAHSJZLTFGGQK-UHFFFAOYSA-N

Formula: C16H27NO4

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

Mol. weight [g/mol]: 297.39

Physical Properties

Property code	Value	Unit	Source
gf	-175.71	kJ/mol	Joback Method
hf	-608.55	kJ/mol	Joback Method
hfus	34.23	kJ/mol	Joback Method
hvap	74.39	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.335		Crippen Method
mcvol	246.000	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	1989.00		NIST Webbook
rinpol	1989.00		NIST Webbook
tb	780.43	K	Joback Method
tc	981.61	K	Joback Method
tf	500.10	K	Joback Method
vc	0.934	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.72	J/mol×K	780.43	Joback Method
cpg	772.94	J/mol×K	813.96	Joback Method
cpg	789.49	J/mol×K	847.49	Joback Method
cpg	805.46	J/mol×K	881.02	Joback Method
cpg	820.94	J/mol×K	914.55	Joback Method
cpg	836.02	J/mol×K	948.08	Joback Method
cpg	850.81	J/mol×K	981.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392593&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

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