1-Aminocyclopentanecarboxylic acid, N-(vinyloxycarbonyl)-, hexyl ester

Inchi: InChI=1S/C15H25NO4/c1-3-5-6-9-12-20-13(17)15(10-7-8-11-15)16-14(18)19-4-2/h4H,2-

InchiKey: XXJLLNUGPOLLAU-UHFFFAOYSA-N

Formula: C15H25NO4

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

Mol. weight [g/mol]: 283.36

Physical Properties

Property code	Value	Unit	Source
hf	-608.60	kJ/mol	Joback Method
hvap	79.06	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.497		Crippen Method
mcvol	231.910	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	1895.00		NIST Webbook
rinpol	1895.00		NIST Webbook
tb	822.25	K	Joback Method
tc	1025.54	K	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=U392606&Units=SI

Legend

hf: Enthalpy of formation 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