1-Aminocyclopentanecarboxylic acid, 3-chloropropoxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C14H24ClNO4/c1-11(2)10-20-12(17)14(6-3-4-7-14)16-13(18)19-9-5-8-15/h11H

InchiKey: HLHCUHZTRVHYFG-UHFFFAOYSA-N

Formula: C14H24ClNO4

SMILES: CC(C)COC(=O)C1(NC(=O)OCCCCl)CCCC1

Mol. weight [g/mol]: 305.80

Physical Properties

Property code	Value	Unit	Source
gf	-294.76	kJ/mol	Joback Method
hf	-713.72	kJ/mol	Joback Method
hfus	31.00	kJ/mol	Joback Method
hvap	74.61	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.853		Crippen Method
mcvol	234.360	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	2054.00		NIST Webbook
rinpol	2054.00		NIST Webbook
tb	774.98	K	Joback Method
tc	982.96	K	Joback Method
tf	494.24	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.68	J/mol×K	774.98	Joback Method
cpg	712.95	J/mol×K	809.64	Joback Method
cpg	728.55	J/mol×K	844.31	Joback Method
cpg	743.58	J/mol×K	878.97	Joback Method
cpg	758.14	J/mol×K	913.63	Joback Method
cpg	772.31	J/mol×K	948.30	Joback Method
cpg	786.21	J/mol×K	982.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392623&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