1-Aminocyclopentanecarboxylic acid, N-(2-chloroethoxycarbonyl)-, pentyl ester

Inchi: InChI=1S/C14H24ClNO4/c1-2-3-6-10-19-12(17)14(7-4-5-8-14)16-13(18)20-11-9-15/h2-1

InchiKey: KIOBOKGWFUAANC-UHFFFAOYSA-N

Formula: C14H24ClNO4

SMILES: CCCCCOC(=O)C1(NC(=O)OCCCl)CCCC1

Mol. weight [g/mol]: 305.80

Physical Properties

Property code	Value	Unit	Source
gf	-292.32	kJ/mol	Joback Method
hf	-708.44	kJ/mol	Joback Method
hfus	34.52	kJ/mol	Joback Method
hvap	75.00	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.998		Crippen Method
mcvol	234.360	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	2057.00		NIST Webbook
rinpol	2057.00		NIST Webbook
tb	775.42	K	Joback Method
tc	980.53	K	Joback Method
tf	509.24	K	Joback Method
vc	0.890	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.14	J/mol×K	775.42	Joback Method
cpg	712.18	J/mol×K	809.60	Joback Method
cpg	727.59	J/mol×K	843.79	Joback Method
cpg	742.44	J/mol×K	877.97	Joback Method
cpg	756.85	J/mol×K	912.16	Joback Method
cpg	770.89	J/mol×K	946.34	Joback Method
cpg	784.66	J/mol×K	980.53	Joback Method

Sources

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=U392550&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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