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

Inchi: InChI=1S/C13H22ClNO4/c1-2-3-9-18-11(16)13(6-4-5-7-13)15-12(17)19-10-8-14/h2-10H2

InchiKey: ZJLONBCFVZGRHI-UHFFFAOYSA-N

Formula: C13H22ClNO4

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

Mol. weight [g/mol]: 291.77

Physical Properties

Property code	Value	Unit	Source
gf	-300.74	kJ/mol	Joback Method
hf	-687.80	kJ/mol	Joback Method
hfus	31.93	kJ/mol	Joback Method
hvap	72.77	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.607		Crippen Method
mcvol	220.270	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	1962.00		NIST Webbook
rinpol	1962.00		NIST Webbook
tb	752.54	K	Joback Method
tc	959.42	K	Joback Method
tf	497.97	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.15	J/mol×K	752.54	Joback Method
cpg	655.70	J/mol×K	787.02	Joback Method
cpg	670.59	J/mol×K	821.50	Joback Method
cpg	684.93	J/mol×K	855.98	Joback Method
cpg	698.80	J/mol×K	890.46	Joback Method
cpg	712.30	J/mol×K	924.94	Joback Method
cpg	725.52	J/mol×K	959.42	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=U392549&Units=SI

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