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

Inchi: InChI=1S/C13H22ClNO4/c1-10(2)9-19-11(16)13(5-3-4-6-13)15-12(17)18-8-7-14/h10H,3-

InchiKey: RWNJIUTUVKLSLG-UHFFFAOYSA-N

Formula: C13H22ClNO4

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

Mol. weight [g/mol]: 291.77

Physical Properties

Property code	Value	Unit	Source
gf	-303.18	kJ/mol	Joback Method
hf	-693.08	kJ/mol	Joback Method
hfus	28.41	kJ/mol	Joback Method
hvap	72.38	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.463		Crippen Method
mcvol	220.270	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
rinpol	1920.00		NIST Webbook
rinpol	1920.00		NIST Webbook
tb	752.10	K	Joback Method
tc	962.15	K	Joback Method
tf	482.97	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.70	J/mol×K	752.10	Joback Method
cpg	656.49	J/mol×K	787.11	Joback Method
cpg	671.60	J/mol×K	822.12	Joback Method
cpg	686.12	J/mol×K	857.12	Joback Method
cpg	700.16	J/mol×K	892.13	Joback Method
cpg	713.81	J/mol×K	927.14	Joback Method
cpg	727.16	J/mol×K	962.15	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=U392556&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