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

Inchi: InChI=1S/C13H20Cl3NO4/c1-9(2)7-20-10(18)12(5-3-4-6-12)17-11(19)21-8-13(14,15)16/h
InchiKey: XEYXNVFWHVRQAC-UHFFFAOYSA-N
Formula: C13H20Cl3NO4
SMILES: CC(C)COC(=O)C1(NC(=O)OCC(Cl)(Cl)Cl)CCCC1
Mol. weight [g/mol]: 360.66

Physical Properties

Property code	Value	Unit	Source
gf	-324.20	kJ/mol	Joback Method
hf	-733.31	kJ/mol	Joback Method
hfus	29.39	kJ/mol	Joback Method
hvap	79.86	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.595		Crippen Method
mcvol	244.750	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	2087.00		NIST Webbook
rinpol	2087.00		NIST Webbook
tb	823.73	K	Joback Method
tc	1049.46	K	Joback Method
tf	545.23	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.41	J/mol×K	823.73	Joback Method
cpg	708.94	J/mol×K	861.35	Joback Method
cpg	722.98	J/mol×K	898.97	Joback Method
cpg	736.68	J/mol×K	936.60	Joback Method
cpg	750.17	J/mol×K	974.22	Joback Method
cpg	763.62	J/mol×K	1011.84	Joback Method
cpg	777.16	J/mol×K	1049.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392537&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

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