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

Inchi: InChI=1S/C12H18Cl3NO4/c1-2-7-19-9(17)11(5-3-4-6-11)16-10(18)20-8-12(13,14)15/h2-8

InchiKey: PHQQYXCUWSDCHC-UHFFFAOYSA-N

Formula: C12H18Cl3NO4

SMILES: CCCOC(=O)C1(NC(=O)OCC(Cl)(Cl)Cl)CCCC1

Mol. weight [g/mol]: 346.63

Physical Properties

Property code	Value	Unit	Source
gf	-330.18	kJ/mol	Joback Method
hf	-707.39	kJ/mol	Joback Method
hfus	30.32	kJ/mol	Joback Method
hvap	78.02	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.349		Crippen Method
mcvol	230.660	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		NIST Webbook
tb	801.29	K	Joback Method
tc	1026.47	K	Joback Method
tf	548.96	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.28	J/mol×K	801.29	Joback Method
cpg	652.04	J/mol×K	838.82	Joback Method
cpg	665.30	J/mol×K	876.35	Joback Method
cpg	678.21	J/mol×K	913.88	Joback Method
cpg	690.90	J/mol×K	951.41	Joback Method
cpg	703.52	J/mol×K	988.94	Joback Method
cpg	716.22	J/mol×K	1026.47	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=U392533&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