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

Inchi: InChI=1S/C14H22Cl3NO4/c1-2-3-6-9-21-11(19)13(7-4-5-8-13)18-12(20)22-10-14(15,16)

InchiKey: NYEMIIDXDXRPNC-UHFFFAOYSA-N

Formula: C14H22Cl3NO4

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

Mol. weight [g/mol]: 374.69

Physical Properties

Property code	Value	Unit	Source
gf	-313.34	kJ/mol	Joback Method
hf	-748.67	kJ/mol	Joback Method
hfus	35.50	kJ/mol	Joback Method
hvap	82.47	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.129		Crippen Method
mcvol	258.840	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	2218.00		NIST Webbook
rinpol	2218.00		NIST Webbook
tb	847.05	K	Joback Method
tc	1067.38	K	Joback Method
tf	571.50	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.51	J/mol×K	847.05	Joback Method
cpg	765.43	J/mol×K	883.77	Joback Method
cpg	779.91	J/mol×K	920.49	Joback Method
cpg	794.09	J/mol×K	957.21	Joback Method
cpg	808.12	J/mol×K	993.94	Joback Method
cpg	822.14	J/mol×K	1030.66	Joback Method
cpg	836.29	J/mol×K	1067.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392535&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