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

Inchi: InChI=1S/C13H20Cl3NO4/c1-2-3-8-20-10(18)12(6-4-5-7-12)17-11(19)21-9-13(14,15)16/h

InchiKey: PHCGUJQTGKLKHC-UHFFFAOYSA-N

Formula: C13H20Cl3NO4

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

Mol. weight [g/mol]: 360.66

Physical Properties

Property code	Value	Unit	Source
gf	-321.76	kJ/mol	Joback Method
hf	-728.03	kJ/mol	Joback Method
hfus	32.91	kJ/mol	Joback Method
hvap	80.25	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	3.739		Crippen Method
mcvol	244.750	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	2127.00		NIST Webbook
rinpol	2127.00		NIST Webbook
tb	824.17	K	Joback Method
tc	1046.61	K	Joback Method
tf	560.23	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.84	J/mol×K	824.17	Joback Method
cpg	708.18	J/mol×K	861.24	Joback Method
cpg	722.05	J/mol×K	898.32	Joback Method
cpg	735.59	J/mol×K	935.39	Joback Method
cpg	748.96	J/mol×K	972.47	Joback Method
cpg	762.28	J/mol×K	1009.54	Joback Method
cpg	775.69	J/mol×K	1046.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392534&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