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

Inchi: InChI=1S/C11H13Cl6NO4/c12-10(13,14)5-21-7(19)9(3-1-2-4-9)18-8(20)22-6-11(15,16)17
InchiKey: WRPUKRDSPDNBKY-UHFFFAOYSA-N
Formula: C11H13Cl6NO4
SMILES: O=C(NC1(C(=O)OCC(Cl)(Cl)Cl)CCCC1)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 435.94

Physical Properties

Property code	Value	Unit	Source
gf	-371.55	kJ/mol	Joback Method
hf	-742.72	kJ/mol	Joback Method
hfus	32.91	kJ/mol	Joback Method
hvap	87.65	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.309		Crippen Method
mcvol	253.290	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	2360.00		NIST Webbook
tb	887.47	K	Joback Method
tc	1134.03	K	Joback Method
tf	629.87	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.83	J/mol×K	887.47	Joback Method
cpg	661.48	J/mol×K	928.56	Joback Method
cpg	673.17	J/mol×K	969.66	Joback Method
cpg	685.10	J/mol×K	1010.75	Joback Method
cpg	697.51	J/mol×K	1051.84	Joback Method
cpg	710.62	J/mol×K	1092.94	Joback Method
cpg	724.66	J/mol×K	1134.03	Joback Method

Sources

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=U392536&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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