1-Aminocyclopentanecarboxylic acid, 3-chloropropoxycarbonyl-, dodecyl ester

Inchi: InChI=1S/C22H40ClNO4/c1-2-3-4-5-6-7-8-9-10-13-18-27-20(25)22(15-11-12-16-22)24-2

InchiKey: AUUIOOQJCQLAAX-UHFFFAOYSA-N

Formula: C22H40ClNO4

SMILES: CCCCCCCCCCCCOC(=O)C1(NC(=O)OCCCCl)CCCC1

Mol. weight [g/mol]: 418.01

Physical Properties

Property code	Value	Unit	Source
gf	-224.96	kJ/mol	Joback Method
hf	-873.56	kJ/mol	Joback Method
hfus	55.24	kJ/mol	Joback Method
hvap	92.81	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	6.118		Crippen Method
mcvol	347.080	ml/mol	McGowan Method
pc	1084.20	kPa	Joback Method
rinpol	2847.00		NIST Webbook
rinpol	2847.00		NIST Webbook
tb	958.46	K	Joback Method
tc	1173.57	K	Joback Method
tf	599.40	K	Joback Method
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1180.98	J/mol×K	958.46	Joback Method
cpg	1201.89	J/mol×K	994.31	Joback Method
cpg	1222.25	J/mol×K	1030.16	Joback Method
cpg	1242.21	J/mol×K	1066.01	Joback Method
cpg	1261.88	J/mol×K	1101.87	Joback Method
cpg	1281.41	J/mol×K	1137.72	Joback Method
cpg	1300.93	J/mol×K	1173.57	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=U392629&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