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

Inchi: InChI=1S/C21H38ClNO4/c1-2-3-4-5-6-7-8-9-12-17-26-19(24)21(14-10-11-15-21)23-20(2

InchiKey: QWYXYEPPPBLLMO-UHFFFAOYSA-N

Formula: C21H38ClNO4

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

Mol. weight [g/mol]: 403.98

Physical Properties

Property code	Value	Unit	Source
gf	-233.38	kJ/mol	Joback Method
hf	-852.92	kJ/mol	Joback Method
hfus	52.65	kJ/mol	Joback Method
hvap	90.58	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.728		Crippen Method
mcvol	332.990	ml/mol	McGowan Method
pc	1156.14	kPa	Joback Method
rinpol	2758.00		NIST Webbook
rinpol	2758.00		NIST Webbook
tb	935.58	K	Joback Method
tc	1146.58	K	Joback Method
tf	588.13	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1117.20	J/mol×K	935.58	Joback Method
cpg	1137.28	J/mol×K	970.75	Joback Method
cpg	1156.81	J/mol×K	1005.91	Joback Method
cpg	1175.91	J/mol×K	1041.08	Joback Method
cpg	1194.69	J/mol×K	1076.25	Joback Method
cpg	1213.28	J/mol×K	1111.42	Joback Method
cpg	1231.80	J/mol×K	1146.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392628&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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