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

Inchi: InChI=1S/C15H26ClNO4/c1-2-3-6-11-20-13(18)15(8-4-5-9-15)17-14(19)21-12-7-10-16/h2

InchiKey: ZJCMRCUOISUGBR-UHFFFAOYSA-N

Formula: C15H26ClNO4

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

Mol. weight [g/mol]: 319.82

Physical Properties

Property code	Value	Unit	Source
gf	-283.90	kJ/mol	Joback Method
hf	-729.08	kJ/mol	Joback Method
hfus	37.11	kJ/mol	Joback Method
hvap	77.22	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.388		Crippen Method
mcvol	248.450	ml/mol	McGowan Method
pc	1787.88	kPa	Joback Method
rinpol	2170.00		NIST Webbook
rinpol	2170.00		NIST Webbook
tb	798.30	K	Joback Method
tc	1002.19	K	Joback Method
tf	520.51	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.27	J/mol×K	798.30	Joback Method
cpg	769.80	J/mol×K	832.28	Joback Method
cpg	785.71	J/mol×K	866.26	Joback Method
cpg	801.08	J/mol×K	900.24	Joback Method
cpg	816.01	J/mol×K	934.23	Joback Method
cpg	830.60	J/mol×K	968.21	Joback Method
cpg	844.93	J/mol×K	1002.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392624&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