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

Inchi: InChI=1S/C18H32ClNO4/c1-2-3-4-5-6-9-14-23-16(21)18(11-7-8-12-18)20-17(22)24-15-1

InchiKey: KYRWVONMXUSQBJ-UHFFFAOYSA-N

Formula: C18H32ClNO4

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

Mol. weight [g/mol]: 361.90

Physical Properties

Property code	Value	Unit	Source
gf	-258.64	kJ/mol	Joback Method
hf	-791.00	kJ/mol	Joback Method
hfus	44.88	kJ/mol	Joback Method
hvap	83.90	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.558		Crippen Method
mcvol	290.720	ml/mol	McGowan Method
pc	1420.78	kPa	Joback Method
rinpol	2459.00		NIST Webbook
rinpol	2459.00		NIST Webbook
tb	866.94	K	Joback Method
tc	1070.99	K	Joback Method
tf	554.32	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.97	J/mol×K	866.94	Joback Method
cpg	949.08	J/mol×K	900.95	Joback Method
cpg	966.58	J/mol×K	934.96	Joback Method
cpg	983.60	J/mol×K	968.96	Joback Method
cpg	1000.23	J/mol×K	1002.97	Joback Method
cpg	1016.57	J/mol×K	1036.98	Joback Method
cpg	1032.73	J/mol×K	1070.99	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=U392626&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