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

Inchi: InChI=1S/C19H34ClNO4/c1-2-3-4-5-6-7-10-15-24-17(22)19(12-8-9-13-19)21-18(23)25-1

InchiKey: BUJMJDMYJLCOIH-UHFFFAOYSA-N

Formula: C19H34ClNO4

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

Mol. weight [g/mol]: 375.93

Physical Properties

Property code	Value	Unit	Source
gf	-250.22	kJ/mol	Joback Method
hf	-811.64	kJ/mol	Joback Method
hfus	47.47	kJ/mol	Joback Method
hvap	86.13	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.948		Crippen Method
mcvol	304.810	ml/mol	McGowan Method
pc	1323.28	kPa	Joback Method
rinpol	2558.00		NIST Webbook
rinpol	2558.00		NIST Webbook
tb	889.82	K	Joback Method
tc	1095.36	K	Joback Method
tf	565.59	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.16	J/mol×K	889.82	Joback Method
cpg	1010.86	J/mol×K	924.08	Joback Method
cpg	1028.97	J/mol×K	958.33	Joback Method
cpg	1046.62	J/mol×K	992.59	Joback Method
cpg	1063.89	J/mol×K	1026.84	Joback Method
cpg	1080.90	J/mol×K	1061.10	Joback Method
cpg	1097.77	J/mol×K	1095.36	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=U392627&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