DL-Alanine, N-methyl-N-(3-chloropropoxycarbonyl)-, decyl ester

Inchi: InChI=1S/C18H34ClNO4/c1-4-5-6-7-8-9-10-11-14-23-17(21)16(2)20(3)18(22)24-15-12-1
InchiKey: SNBHOYQCOKANKM-UHFFFAOYSA-N
Formula: C18H34ClNO4
SMILES: CCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 363.92

Physical Properties

Property code	Value	Unit	Source
gf	-270.75	kJ/mol	Joback Method
hf	-857.94	kJ/mol	Joback Method
hfus	51.64	kJ/mol	Joback Method
hvap	80.01	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.756		Crippen Method
mcvol	301.580	ml/mol	McGowan Method
pc	1201.46	kPa	Joback Method
rinpol	2373.00		NIST Webbook
rinpol	2373.00		NIST Webbook
tb	813.25	K	Joback Method
tc	1000.05	K	Joback Method
tf	484.33	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.11	J/mol×K	813.25	Joback Method
cpg	940.88	J/mol×K	844.38	Joback Method
cpg	956.62	J/mol×K	875.52	Joback Method
cpg	971.37	J/mol×K	906.65	Joback Method
cpg	985.15	J/mol×K	937.79	Joback Method
cpg	997.97	J/mol×K	968.92	Joback Method
cpg	1009.86	J/mol×K	1000.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392782&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