DL-Valine, N-methyl-N-(3-chloropropoxycarbonyl)-, hexadecyl ester

Inchi: InChI=1S/C26H50ClNO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-31-25(29)24(23(2

InchiKey: LKGYUQNLHXSBIM-UHFFFAOYSA-N

Formula: C26H50ClNO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCCCCl

Mol. weight [g/mol]: 476.13

Physical Properties

Property code	Value	Unit	Source
gf	-205.83	kJ/mol	Joback Method
hf	-1028.34	kJ/mol	Joback Method
hfus	68.84	kJ/mol	Joback Method
hvap	97.43	kJ/mol	Joback Method
log10ws	-8.00		Crippen Method
logp	7.733		Crippen Method
mcvol	414.300	ml/mol	McGowan Method
pc	752.67	kPa	Joback Method
rinpol	3121.00		NIST Webbook
rinpol	3121.00		NIST Webbook
tb	995.85	K	Joback Method
tc	1229.80	K	Joback Method
tf	559.49	K	Joback Method
vc	1.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1420.85	J/mol×K	995.85	Joback Method
cpg	1441.19	J/mol×K	1034.84	Joback Method
cpg	1459.71	J/mol×K	1073.83	Joback Method
cpg	1476.48	J/mol×K	1112.82	Joback Method
cpg	1491.57	J/mol×K	1151.82	Joback Method
cpg	1505.07	J/mol×K	1190.81	Joback Method
cpg	1517.05	J/mol×K	1229.80	Joback Method

Sources

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=U392986&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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