DL-Valine, N-methyl-N-hexyloxycarbonyl-, pentyl ester

Inchi: InChI=1S/C18H35NO4/c1-6-8-10-12-14-23-18(21)19(5)16(15(3)4)17(20)22-13-11-9-7-2/h
InchiKey: MZZJVHLIQXVPNN-UHFFFAOYSA-N
Formula: C18H35NO4
SMILES: CCCCCCOC(=O)N(C)C(C(=O)OCCCCC)C(C)C
Mol. weight [g/mol]: 329.47

Physical Properties

Property code	Value	Unit	Source
gf	-261.26	kJ/mol	Joback Method
hf	-847.48	kJ/mol	Joback Method
hfus	43.92	kJ/mol	Joback Method
hvap	75.24	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.393		Crippen Method
mcvol	289.340	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpol	2044.00		NIST Webbook
rinpol	2044.00		NIST Webbook
tb	775.38	K	Joback Method
tc	957.28	K	Joback Method
tf	439.41	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.99	J/mol×K	775.38	Joback Method
cpg	910.82	J/mol×K	805.70	Joback Method
cpg	927.65	J/mol×K	836.01	Joback Method
cpg	943.49	J/mol×K	866.33	Joback Method
cpg	958.38	J/mol×K	896.65	Joback Method
cpg	972.31	J/mol×K	926.96	Joback Method
cpg	985.32	J/mol×K	957.28	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=U392888&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