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

Inchi: InChI=1S/C24H47NO4/c1-6-8-10-12-13-14-15-16-18-19-28-23(26)22(21(3)4)25(5)24(27)

InchiKey: AGNLWSZYFMBGSI-UHFFFAOYSA-N

Formula: C24H47NO4

SMILES: CCCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCCCCCC

Mol. weight [g/mol]: 413.63

Physical Properties

Property code	Value	Unit	Source
gf	-210.74	kJ/mol	Joback Method
hf	-971.32	kJ/mol	Joback Method
hfus	59.46	kJ/mol	Joback Method
hvap	88.60	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.734		Crippen Method
mcvol	373.880	ml/mol	McGowan Method
pc	856.97	kPa	Joback Method
rinpol	2632.00		NIST Webbook
rinpol	2632.00		NIST Webbook
tb	912.66	K	Joback Method
tc	1118.65	K	Joback Method
tf	507.03	K	Joback Method
vc	1.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1263.02	J/mol×K	912.66	Joback Method
cpg	1283.26	J/mol×K	946.99	Joback Method
cpg	1302.04	J/mol×K	981.32	Joback Method
cpg	1319.40	J/mol×K	1015.66	Joback Method
cpg	1335.38	J/mol×K	1049.99	Joback Method
cpg	1350.03	J/mol×K	1084.32	Joback Method
cpg	1363.40	J/mol×K	1118.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392894&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

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