DL-Valyl-DL-valine, N-methyl-N-hexyloxycarbonyl-, hexyl ester

Inchi: InChI=1S/C25H48N2O5/c1-9-11-13-15-17-31-24(29)22(20(5)6)26(7)23(28)21(19(3)4)27(

InchiKey: ZRPSQVNGMCIGSM-UHFFFAOYSA-N

Formula: C25H48N2O5

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

Mol. weight [g/mol]: 456.66

Physical Properties

Property code	Value	Unit	Source
gf	-225.34	kJ/mol	Joback Method
hf	-1047.57	kJ/mol	Joback Method
hfus	59.63	kJ/mol	Joback Method
hvap	98.84	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.266		Crippen Method
mcvol	399.520	ml/mol	McGowan Method
pc	847.51	kPa	Joback Method
rinpol	2705.00		NIST Webbook
rinpol	2705.00		NIST Webbook
tb	1000.97	K	Joback Method
tc	1232.10	K	Joback Method
tf	570.70	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1391.87	J/mol×K	1000.97	Joback Method
cpg	1410.74	J/mol×K	1039.49	Joback Method
cpg	1427.82	J/mol×K	1078.01	Joback Method
cpg	1443.18	J/mol×K	1116.53	Joback Method
cpg	1456.92	J/mol×K	1155.06	Joback Method
cpg	1469.09	J/mol×K	1193.58	Joback Method
cpg	1479.78	J/mol×K	1232.10	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=U392898&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