DL-Valyl-DL-Valine, N,N'-dimethyl-N'-vinyloxycarbonyl-, pentyl ester

Inchi: InChI=1S/C20H36N2O5/c1-9-11-12-13-27-19(24)17(15(5)6)21(7)18(23)16(14(3)4)22(8)2

InchiKey: LYQKPQFXPHEWRG-UHFFFAOYSA-N

Formula: C20H36N2O5

SMILES: C=COC(=O)N(C)C(C(=O)N(C)C(C(=O)OCCCCC)C(C)C)C(C)C

Mol. weight [g/mol]: 384.51

Physical Properties

Property code	Value	Unit	Source
gf	-179.60	kJ/mol	Joback Method
hf	-818.94	kJ/mol	Joback Method
hfus	45.40	kJ/mol	Joback Method
hvap	87.04	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.439		Crippen Method
mcvol	324.770	ml/mol	McGowan Method
pc	1178.47	kPa	Joback Method
rinpol	2198.00		NIST Webbook
rinpol	2198.00		NIST Webbook
tb	883.25	K	Joback Method
tc	1083.16	K	Joback Method
tf	512.59	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1051.98	J/mol×K	883.25	Joback Method
cpg	1068.59	J/mol×K	916.57	Joback Method
cpg	1083.98	J/mol×K	949.89	Joback Method
cpg	1098.18	J/mol×K	983.21	Joback Method
cpg	1111.24	J/mol×K	1016.52	Joback Method
cpg	1123.20	J/mol×K	1049.84	Joback Method
cpg	1134.09	J/mol×K	1083.16	Joback Method

Sources

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=U392973&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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