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

Inchi: InChI=1S/C21H38N2O5/c1-9-11-12-13-14-28-20(25)18(16(5)6)22(7)19(24)17(15(3)4)23(
InchiKey: ZZLHPVNIRJUUBT-UHFFFAOYSA-N
Formula: C21H38N2O5
SMILES: C=COC(=O)N(C)C(C(=O)N(C)C(C(=O)OCCCCCC)C(C)C)C(C)C
Mol. weight [g/mol]: 398.54

Physical Properties

Property code	Value	Unit	Source
gf	-171.18	kJ/mol	Joback Method
hf	-839.58	kJ/mol	Joback Method
hfus	47.99	kJ/mol	Joback Method
hvap	89.26	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.829		Crippen Method
mcvol	338.860	ml/mol	McGowan Method
pc	1104.47	kPa	Joback Method
rinpol	2297.00		NIST Webbook
rinpol	2297.00		NIST Webbook
tb	906.13	K	Joback Method
tc	1109.80	K	Joback Method
tf	523.86	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1112.88	J/mol×K	906.13	Joback Method
cpg	1129.78	J/mol×K	940.08	Joback Method
cpg	1145.39	J/mol×K	974.02	Joback Method
cpg	1159.76	J/mol×K	1007.97	Joback Method
cpg	1172.93	J/mol×K	1041.91	Joback Method
cpg	1184.94	J/mol×K	1075.86	Joback Method
cpg	1195.84	J/mol×K	1109.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392974&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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