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

Inchi: InChI=1S/C23H42N2O5/c1-9-11-12-13-14-15-16-30-22(27)20(18(5)6)24(7)21(26)19(17(3
InchiKey: AZSKSRRPAYNWDJ-UHFFFAOYSA-N
Formula: C23H42N2O5
SMILES: C=COC(=O)N(C)C(C(=O)N(C)C(C(=O)OCCCCCCCC)C(C)C)C(C)C
Mol. weight [g/mol]: 426.59

Physical Properties

Property code	Value	Unit	Source
gf	-154.34	kJ/mol	Joback Method
hf	-880.86	kJ/mol	Joback Method
hfus	53.17	kJ/mol	Joback Method
hvap	93.71	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.610		Crippen Method
mcvol	367.040	ml/mol	McGowan Method
pc	975.95	kPa	Joback Method
rinpol	2507.00		NIST Webbook
rinpol	2507.00		NIST Webbook
tb	951.89	K	Joback Method
tc	1165.93	K	Joback Method
tf	546.40	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1236.34	J/mol×K	951.89	Joback Method
cpg	1253.90	J/mol×K	987.56	Joback Method
cpg	1270.01	J/mol×K	1023.24	Joback Method
cpg	1284.72	J/mol×K	1058.91	Joback Method
cpg	1298.10	J/mol×K	1094.59	Joback Method
cpg	1310.21	J/mol×K	1130.26	Joback Method
cpg	1321.09	J/mol×K	1165.93	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=U392975&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