DL-Valyl-DL-valine, N-methyl-N-(but-3-en-1-yloxycarbonyl)-, but-3-en-1-yl ester

Inchi: InChI=1S/C21H36N2O5/c1-9-11-13-27-20(25)18(16(5)6)22(7)19(24)17(15(3)4)23(8)21(2

InchiKey: YGQCTRYPHPMJDM-UHFFFAOYSA-N

Formula: C21H36N2O5

SMILES: C=CCCOC(=O)C(C(C)C)N(C)C(=O)C(C(C)C)N(C)C(=O)OCCC=C

Mol. weight [g/mol]: 396.52

Physical Properties

Property code	Value	Unit	Source
gf	-83.34	kJ/mol	Joback Method
hf	-714.15	kJ/mol	Joback Method
hfus	46.71	kJ/mol	Joback Method
hvap	88.59	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.258		Crippen Method
mcvol	334.560	ml/mol	McGowan Method
pc	1135.96	kPa	Joback Method
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook
tb	902.81	K	Joback Method
tc	1106.27	K	Joback Method
tf	522.10	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.23	J/mol×K	902.81	Joback Method
cpg	1100.63	J/mol×K	936.72	Joback Method
cpg	1115.80	J/mol×K	970.63	Joback Method
cpg	1129.79	J/mol×K	1004.54	Joback Method
cpg	1142.65	J/mol×K	1038.45	Joback Method
cpg	1154.42	J/mol×K	1072.36	Joback Method
cpg	1165.15	J/mol×K	1106.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392972&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