DL-Valine, N-methyl-N-(but-3-en-1-yloxycarbonyl)-, nonyl ester

Inchi: InChI=1S/C20H37NO4/c1-6-8-10-11-12-13-14-16-24-19(22)18(17(3)4)21(5)20(23)25-15-

InchiKey: WBGUJXSSWRZEHK-UHFFFAOYSA-N

Formula: C20H37NO4

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

Mol. weight [g/mol]: 355.51

Physical Properties

Property code	Value	Unit	Source
gf	-156.58	kJ/mol	Joback Method
hf	-763.33	kJ/mol	Joback Method
hfus	47.82	kJ/mol	Joback Method
hvap	79.02	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.949		Crippen Method
mcvol	313.220	ml/mol	McGowan Method
pc	1118.56	kPa	Joback Method
rinpol	2259.00		NIST Webbook
rinpol	2259.00		NIST Webbook
tb	817.82	K	Joback Method
tc	1004.78	K	Joback Method
tf	460.19	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	986.33	J/mol×K	817.82	Joback Method
cpg	1004.33	J/mol×K	848.98	Joback Method
cpg	1021.26	J/mol×K	880.14	Joback Method
cpg	1037.13	J/mol×K	911.30	Joback Method
cpg	1051.97	J/mol×K	942.46	Joback Method
cpg	1065.82	J/mol×K	973.62	Joback Method
cpg	1078.69	J/mol×K	1004.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392961&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