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

Inchi: InChI=1S/C15H25NO4/c1-6-8-10-19-14(17)13(12(3)4)16(5)15(18)20-11-9-7-2/h6-7,12-13
InchiKey: AYHDDZISXLTWAD-UHFFFAOYSA-N
Formula: C15H25NO4
SMILES: C=CCCOC(=O)C(C(C)C)N(C)C(=O)OCCC=C
Mol. weight [g/mol]: 283.36

Physical Properties

Property code	Value	Unit	Source
gf	-110.84	kJ/mol	Joback Method
hf	-534.70	kJ/mol	Joback Method
hfus	33.59	kJ/mol	Joback Method
hvap	67.22	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.775		Crippen Method
mcvol	238.470	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	1782.00		NIST Webbook
rinpol	1782.00		NIST Webbook
tb	700.10	K	Joback Method
tc	883.75	K	Joback Method
tf	402.08	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.69	J/mol×K	700.10	Joback Method
cpg	686.43	J/mol×K	730.71	Joback Method
cpg	701.31	J/mol×K	761.32	Joback Method
cpg	715.37	J/mol×K	791.93	Joback Method
cpg	728.61	J/mol×K	822.54	Joback Method
cpg	741.05	J/mol×K	853.15	Joback Method
cpg	752.72	J/mol×K	883.75	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=U392971&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