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

Inchi: InChI=1S/C28H53NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-21-22-24-32-27(30)26
Inchikey: HRPBNPCGWNWHBN-UHFFFAOYSA-N
Formula: C28H53NO4
SMILES: C=CCCOC(=O)N(C)C(C(=O)OCCCCCCCCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 467.72

Physical Properties

Property code	Value	Unit	Source
gf	-89.22	kJ/mol	Joback Method
hf	-928.45	kJ/mol	Joback Method
hfus	68.55	kJ/mol	Joback Method
hvap	96.83	kJ/mol	Joback Method
log10ws	-8.54		Crippen Method
logp	8.070		Crippen Method
mcvol	425.940	ml/mol	McGowan Method
pc	708.09	kPa	Joback Method
rinpol	3066.00		NIST Webbook
rinpol	3066.00		NIST Webbook
tb	1000.86	K	Joback Method
tc	1239.79	K	Joback Method
tf	550.35	K	Joback Method
vc	1.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1490.00	J/mol×K	1000.86	Joback Method
cpg	1511.97	J/mol×K	1040.68	Joback Method
cpg	1532.02	J/mol×K	1080.50	Joback Method
cpg	1550.23	J/mol×K	1120.33	Joback Method
cpg	1566.70	J/mol×K	1160.15	Joback Method
cpg	1581.53	J/mol×K	1199.97	Joback Method
cpg	1594.81	J/mol×K	1239.79	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=U392969&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