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

Inchi: InChI=1S/C26H49NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-22-30-25(28)24(23(3)4
InchiKey: ZZIPTHAWGQRJTL-UHFFFAOYSA-N
Formula: C26H49NO4
SMILES: C=CCCOC(=O)N(C)C(C(=O)OCCCCCCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 439.67

Physical Properties

Property code	Value	Unit	Source
gf	-106.06	kJ/mol	Joback Method
hf	-887.17	kJ/mol	Joback Method
hfus	63.37	kJ/mol	Joback Method
hvap	92.38	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	7.290		Crippen Method
mcvol	397.760	ml/mol	McGowan Method
pc	786.39	kPa	Joback Method
rinpol	2859.00		NIST Webbook
rinpol	2859.00		NIST Webbook
tb	955.10	K	Joback Method
tc	1174.45	K	Joback Method
tf	527.81	K	Joback Method
vc	1.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1361.12	J/mol×K	955.10	Joback Method
cpg	1381.83	J/mol×K	991.66	Joback Method
cpg	1400.92	J/mol×K	1028.22	Joback Method
cpg	1418.46	J/mol×K	1064.78	Joback Method
cpg	1434.50	J/mol×K	1101.33	Joback Method
cpg	1449.13	J/mol×K	1137.89	Joback Method
cpg	1462.40	J/mol×K	1174.45	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=U392967&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