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

InchI: InChI=1S/C24H45NO4/c1-6-8-10-11-12-13-14-15-16-17-18-20-28-23(26)22(21(3)4)25(5)
InchiKey: POINDAUGJXAJJM-UHFFFAOYSA-N
Formula: C24H45NO4
SMILES: C=CCCOC(=O)N(C)C(C(=O)OCCCCCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 411.62

Physical Properties

Property code	Value	Unit	Source
gf	-122.90	kJ/mol	Joback Method
hf	-845.89	kJ/mol	Joback Method
hfus	58.18	kJ/mol	Joback Method
hvap	87.93	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.510		Crippen Method
mcvol	369.580	ml/mol	McGowan Method
pc	878.44	kPa	Joback Method
rinpol	2663.00		NIST Webbook
rinpol	2663.00		NIST Webbook
tb	909.34	K	Joback Method
tc	1113.95	K	Joback Method
tf	505.27	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1233.93	J/mol×K	909.34	Joback Method
cpg	1253.59	J/mol×K	943.44	Joback Method
cpg	1271.85	J/mol×K	977.54	Joback Method
cpg	1288.78	J/mol×K	1011.64	Joback Method
cpg	1304.41	J/mol×K	1045.74	Joback Method
cpg	1318.79	J/mol×K	1079.85	Joback Method
cpg	1331.98	J/mol×K	1113.95	Joback Method

Sources

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=U392965&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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