DL-Valine, N-methyl-N-(2-ethylhexyloxycarbonyl)-, tetradecyl ester

Inchi: InChI=1S/C29H57NO4/c1-7-10-12-13-14-15-16-17-18-19-20-21-23-33-28(31)27(25(4)5)3
InchiKey: RUTJAPWWXGBBDF-UHFFFAOYSA-N
Formula: C29H57NO4
SMILES: CCCCCCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 483.77

Physical Properties

Property code	Value	Unit	Source
gf	-171.08	kJ/mol	Joback Method
hf	-1079.80	kJ/mol	Joback Method
hfus	68.89	kJ/mol	Joback Method
hvap	99.34	kJ/mol	Joback Method
log10ws	-8.86		Crippen Method
logp	8.540		Crippen Method
mcvol	444.330	ml/mol	McGowan Method
pc	661.53	kPa	Joback Method
rinpol	3027.00		NIST Webbook
rinpol	3027.00		NIST Webbook
tb	1026.62	K	Joback Method
tc	1278.67	K	Joback Method
tf	548.38	K	Joback Method
vc	1.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1585.94	J/mol×K	1026.62	Joback Method
cpg	1608.93	J/mol×K	1068.63	Joback Method
cpg	1629.66	J/mol×K	1110.64	Joback Method
cpg	1648.23	J/mol×K	1152.64	Joback Method
cpg	1664.77	J/mol×K	1194.65	Joback Method
cpg	1679.36	J/mol×K	1236.66	Joback Method
cpg	1692.13	J/mol×K	1278.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392918&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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