DL-Valine, N-methyl-N-decyloxycarbonyl-, pentadecyl ester

Inchi: InChI=1S/C32H63NO4/c1-6-8-10-12-14-16-17-18-19-20-22-23-25-27-36-31(34)30(29(3)4
InchiKey: CGLVEMAEYJUCCX-UHFFFAOYSA-N
Formula: C32H63NO4
SMILES: CCCCCCCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCCCCCCCCCC
Mol. weight [g/mol]: 525.85

Physical Properties

Property code	Value	Unit	Source
gf	-143.38	kJ/mol	Joback Method
hf	-1136.44	kJ/mol	Joback Method
hfus	80.19	kJ/mol	Joback Method
hvap	106.41	kJ/mol	Joback Method
log10ws	-10.36		Crippen Method
logp	9.854		Crippen Method
mcvol	486.600	ml/mol	McGowan Method
pc	571.24	kPa	Joback Method
rinpol	3431.00		NIST Webbook
rinpol	3431.00		NIST Webbook
tb	1095.70	K	Joback Method
tc	1398.14	K	Joback Method
tf	597.19	K	Joback Method
vc	1.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1782.81	J/mol×K	1095.70	Joback Method
cpg	1808.62	J/mol×K	1146.11	Joback Method
cpg	1831.28	J/mol×K	1196.51	Joback Method
cpg	1851.00	J/mol×K	1246.92	Joback Method
cpg	1868.01	J/mol×K	1297.33	Joback Method
cpg	1882.51	J/mol×K	1347.74	Joback Method
cpg	1894.71	J/mol×K	1398.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392932&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

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