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

Inchi: InChI=1S/C33H65NO4/c1-6-8-10-12-14-16-17-18-19-20-21-23-24-26-28-37-32(35)31(30

InchiKey: MTNVFLJYJURKLD-UHFFFAOYSA-N

Formula: C33H65NO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCCCCCCCCCC

Mol. weight [g/mol]: 539.87

Physical Properties

Property code	Value	Unit	Source
gf	-134.96	kJ/mol	Joback Method
hf	-1157.08	kJ/mol	Joback Method
hfus	82.78	kJ/mol	Joback Method
hvap	108.63	kJ/mol	Joback Method
log10ws	-10.78		Crippen Method
logp	10.245		Crippen Method
mcvol	500.690	ml/mol	McGowan Method
pc	545.90	kPa	Joback Method
rinpol	3536.00		NIST Webbook
rinpol	3536.00		NIST Webbook
tb	1118.58	K	Joback Method
tc	1440.64	K	Joback Method
tf	608.46	K	Joback Method
vc	1.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1848.87	J/mol×K	1118.58	Joback Method
cpg	1875.62	J/mol×K	1172.26	Joback Method
cpg	1898.86	J/mol×K	1225.93	Joback Method
cpg	1918.84	J/mol×K	1279.61	Joback Method
cpg	1935.85	J/mol×K	1333.29	Joback Method
cpg	1950.14	J/mol×K	1386.97	Joback Method
cpg	1962.00	J/mol×K	1440.64	Joback Method

Sources

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=U392933&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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