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

Inchi: InChI=1S/C30H59NO4/c1-6-8-10-12-14-16-17-18-20-21-23-25-34-29(32)28(27(3)4)31(5)
InchiKey: ARBNBXYHDQEREA-UHFFFAOYSA-N
Formula: C30H59NO4
SMILES: CCCCCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCCCCCCCCCC
Mol. weight [g/mol]: 497.79

Physical Properties

Property code	Value	Unit	Source
gf	-160.22	kJ/mol	Joback Method
hf	-1095.16	kJ/mol	Joback Method
hfus	75.00	kJ/mol	Joback Method
hvap	101.95	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	9.074		Crippen Method
mcvol	458.420	ml/mol	McGowan Method
pc	627.51	kPa	Joback Method
rinpol	3224.00		NIST Webbook
rinpol	3224.00		NIST Webbook
tb	1049.94	K	Joback Method
tc	1319.00	K	Joback Method
tf	574.65	K	Joback Method
vc	1.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1651.20	J/mol×K	1049.94	Joback Method
cpg	1675.29	J/mol×K	1094.78	Joback Method
cpg	1696.85	J/mol×K	1139.63	Joback Method
cpg	1716.00	J/mol×K	1184.47	Joback Method
cpg	1732.89	J/mol×K	1229.31	Joback Method
cpg	1747.65	J/mol×K	1274.16	Joback Method
cpg	1760.41	J/mol×K	1319.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392930&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