DL-Valine, N-methyl-N-octyloxycarbonyl-, tetradecyl ester

Inchi: InChI=1S/C29H57NO4/c1-6-8-10-12-14-15-16-17-18-19-21-22-24-33-28(31)27(26(3)4)30

InchiKey: ONLNNGXCOYPWMM-UHFFFAOYSA-N

Formula: C29H57NO4

SMILES: CCCCCCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCCCCCCCC

Mol. weight [g/mol]: 483.77

Physical Properties

Property code	Value	Unit	Source
gf	-168.64	kJ/mol	Joback Method
hf	-1074.52	kJ/mol	Joback Method
hfus	72.41	kJ/mol	Joback Method
hvap	99.73	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.684		Crippen Method
mcvol	444.330	ml/mol	McGowan Method
pc	658.81	kPa	Joback Method
rinpol	3126.00		NIST Webbook
rinpol	3126.00		NIST Webbook
tb	1027.06	K	Joback Method
tc	1282.05	K	Joback Method
tf	563.38	K	Joback Method
vc	1.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1585.71	J/mol×K	1027.06	Joback Method
cpg	1609.03	J/mol×K	1069.56	Joback Method
cpg	1630.06	J/mol×K	1112.06	Joback Method
cpg	1648.91	J/mol×K	1154.56	Joback Method
cpg	1665.69	J/mol×K	1197.05	Joback Method
cpg	1680.51	J/mol×K	1239.55	Joback Method
cpg	1693.49	J/mol×K	1282.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392910&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