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

Inchi: InChI=1S/C25H49NO4/c1-6-8-10-12-14-15-17-18-20-29-24(27)23(22(3)4)26(5)25(28)30-

InchiKey: GJIPEYQMZFSGNN-UHFFFAOYSA-N

Formula: C25H49NO4

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

Mol. weight [g/mol]: 427.66

Physical Properties

Property code	Value	Unit	Source
gf	-202.32	kJ/mol	Joback Method
hf	-991.96	kJ/mol	Joback Method
hfus	62.05	kJ/mol	Joback Method
hvap	90.82	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	7.124		Crippen Method
mcvol	387.970	ml/mol	McGowan Method
pc	810.76	kPa	Joback Method
rinpol	2722.00		NIST Webbook
rinpol	2722.00		NIST Webbook
tb	935.54	K	Joback Method
tc	1148.84	K	Joback Method
tf	518.30	K	Joback Method
vc	1.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1326.77	J/mol×K	935.54	Joback Method
cpg	1347.53	J/mol×K	971.09	Joback Method
cpg	1366.71	J/mol×K	1006.64	Joback Method
cpg	1384.35	J/mol×K	1042.19	Joback Method
cpg	1400.51	J/mol×K	1077.74	Joback Method
cpg	1415.24	J/mol×K	1113.29	Joback Method
cpg	1428.60	J/mol×K	1148.84	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=U392906&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