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

Inchi: InChI=1S/C23H45NO4/c1-6-8-10-12-14-16-18-27-22(25)21(20(3)4)24(5)23(26)28-19-17-

InchiKey: KVVLDHIUUGDCQA-UHFFFAOYSA-N

Formula: C23H45NO4

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

Mol. weight [g/mol]: 399.61

Physical Properties

Property code	Value	Unit	Source
gf	-219.16	kJ/mol	Joback Method
hf	-950.68	kJ/mol	Joback Method
hfus	56.88	kJ/mol	Joback Method
hvap	86.37	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	6.344		Crippen Method
mcvol	359.790	ml/mol	McGowan Method
pc	907.24	kPa	Joback Method
rinpol	2523.00		NIST Webbook
rinpol	2523.00		NIST Webbook
tb	889.78	K	Joback Method
tc	1089.53	K	Joback Method
tf	495.76	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1199.76	J/mol×K	889.78	Joback Method
cpg	1219.52	J/mol×K	923.07	Joback Method
cpg	1237.93	J/mol×K	956.36	Joback Method
cpg	1255.02	J/mol×K	989.65	Joback Method
cpg	1270.82	J/mol×K	1022.95	Joback Method
cpg	1285.38	J/mol×K	1056.24	Joback Method
cpg	1298.73	J/mol×K	1089.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392904&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