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

Inchi: InChI=1S/C20H39NO4/c1-6-8-10-11-12-14-16-25-20(23)21(5)18(17(3)4)19(22)24-15-13-

InchiKey: YURDBXKQVXICCX-UHFFFAOYSA-N

Formula: C20H39NO4

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

Mol. weight [g/mol]: 357.53

Physical Properties

Property code	Value	Unit	Source
gf	-244.42	kJ/mol	Joback Method
hf	-888.76	kJ/mol	Joback Method
hfus	49.10	kJ/mol	Joback Method
hvap	79.69	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	5.173		Crippen Method
mcvol	317.520	ml/mol	McGowan Method
pc	1087.78	kPa	Joback Method
rinpol	2229.00		NIST Webbook
rinpol	2229.00		NIST Webbook
tb	821.14	K	Joback Method
tc	1007.78	K	Joback Method
tf	461.95	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.53	J/mol×K	821.14	Joback Method
cpg	1032.07	J/mol×K	852.25	Joback Method
cpg	1049.49	J/mol×K	883.35	Joback Method
cpg	1065.82	J/mol×K	914.46	Joback Method
cpg	1081.08	J/mol×K	945.57	Joback Method
cpg	1095.30	J/mol×K	976.68	Joback Method
cpg	1108.50	J/mol×K	1007.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392901&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