DL-Valine, N-methyl-N-(2-ethylhexyloxycarbonyl)-, octyl ester

Inchi: InChI=1S/C23H45NO4/c1-7-10-12-13-14-15-17-27-22(25)21(19(4)5)24(6)23(26)28-18-20

InchiKey: XESGSZHBNHJFEU-UHFFFAOYSA-N

Formula: C23H45NO4

SMILES: CCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCC(CC)CCCC

Mol. weight [g/mol]: 399.61

Physical Properties

Property code	Value	Unit	Source
gf	-221.60	kJ/mol	Joback Method
hf	-955.96	kJ/mol	Joback Method
hfus	53.35	kJ/mol	Joback Method
hvap	85.98	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	6.200		Crippen Method
mcvol	359.790	ml/mol	McGowan Method
pc	911.63	kPa	Joback Method
rinpol	2423.00		NIST Webbook
rinpol	2423.00		NIST Webbook
tb	889.34	K	Joback Method
tc	1088.83	K	Joback Method
tf	480.76	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1200.19	J/mol×K	889.34	Joback Method
cpg	1219.91	J/mol×K	922.59	Joback Method
cpg	1238.27	J/mol×K	955.84	Joback Method
cpg	1255.29	J/mol×K	989.08	Joback Method
cpg	1271.03	J/mol×K	1022.33	Joback Method
cpg	1285.52	J/mol×K	1055.58	Joback Method
cpg	1298.79	J/mol×K	1088.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392912&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