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

Inchi: InChI=1S/C26H51NO4/c1-7-10-12-13-14-15-16-17-18-20-30-25(28)24(22(4)5)27(6)26(29
InchiKey: YYGWYCUOHYVPMO-UHFFFAOYSA-N
Formula: C26H51NO4
SMILES: CCCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 441.69

Physical Properties

Property code	Value	Unit	Source
gf	-196.34	kJ/mol	Joback Method
hf	-1017.88	kJ/mol	Joback Method
hfus	61.12	kJ/mol	Joback Method
hvap	92.66	kJ/mol	Joback Method
log10ws	-7.61		Crippen Method
logp	7.370		Crippen Method
mcvol	402.060	ml/mol	McGowan Method
pc	771.60	kPa	Joback Method
rinpol	2723.00		NIST Webbook
rinpol	2723.00		NIST Webbook
tb	957.98	K	Joback Method
tc	1178.26	K	Joback Method
tf	514.57	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1391.31	J/mol×K	957.98	Joback Method
cpg	1412.46	J/mol×K	994.69	Joback Method
cpg	1431.89	J/mol×K	1031.41	Joback Method
cpg	1449.66	J/mol×K	1068.12	Joback Method
cpg	1465.84	J/mol×K	1104.83	Joback Method
cpg	1480.48	J/mol×K	1141.54	Joback Method
cpg	1493.65	J/mol×K	1178.26	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392915&Units=SI

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