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

Inchi: InChI=1S/C27H53NO4/c1-7-10-12-13-14-15-16-17-18-19-21-31-26(29)25(23(4)5)28(6)27

InchiKey: VBJSNIFZNZICRE-UHFFFAOYSA-N

Formula: C27H53NO4

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

Mol. weight [g/mol]: 455.71

Physical Properties

Property code	Value	Unit	Source
gf	-187.92	kJ/mol	Joback Method
hf	-1038.52	kJ/mol	Joback Method
hfus	63.71	kJ/mol	Joback Method
hvap	94.89	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	7.760		Crippen Method
mcvol	416.150	ml/mol	McGowan Method
pc	732.04	kPa	Joback Method
rinpol	2824.00		NIST Webbook
rinpol	2824.00		NIST Webbook
tb	980.86	K	Joback Method
tc	1210.38	K	Joback Method
tf	525.84	K	Joback Method
vc	1.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1455.86	J/mol×K	980.86	Joback Method
cpg	1477.58	J/mol×K	1019.11	Joback Method
cpg	1497.41	J/mol×K	1057.37	Joback Method
cpg	1515.45	J/mol×K	1095.62	Joback Method
cpg	1531.76	J/mol×K	1133.87	Joback Method
cpg	1546.42	J/mol×K	1172.13	Joback Method
cpg	1559.49	J/mol×K	1210.38	Joback Method

Sources

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=U392916&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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