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

Inchi: InChI=1S/C28H55NO4/c1-6-8-10-12-14-15-16-17-18-20-21-23-32-27(30)26(25(3)4)29(5)
InchiKey: UZSCLFPTAWKOBE-UHFFFAOYSA-N
Formula: C28H55NO4
SMILES: CCCCCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCCCCCCCC
Mol. weight [g/mol]: 469.74

Physical Properties

Property code	Value	Unit	Source
gf	-177.06	kJ/mol	Joback Method
hf	-1053.88	kJ/mol	Joback Method
hfus	69.82	kJ/mol	Joback Method
hvap	97.50	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	8.294		Crippen Method
mcvol	430.240	ml/mol	McGowan Method
pc	692.52	kPa	Joback Method
rinpol	3019.00		NIST Webbook
rinpol	3019.00		NIST Webbook
tb	1004.18	K	Joback Method
tc	1246.68	K	Joback Method
tf	552.11	K	Joback Method
vc	1.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.48	J/mol×K	1004.18	Joback Method
cpg	1543.09	J/mol×K	1044.60	Joback Method
cpg	1563.61	J/mol×K	1085.01	Joback Method
cpg	1582.16	J/mol×K	1125.43	Joback Method
cpg	1598.80	J/mol×K	1165.84	Joback Method
cpg	1613.65	J/mol×K	1206.26	Joback Method
cpg	1626.78	J/mol×K	1246.68	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=U392909&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