DL-Valyl-DL-valine, N-methyl-N-octyloxycarbonyl-, octyl ester

Inchi: InChI=1S/C29H56N2O5/c1-9-11-13-15-17-19-21-35-28(33)26(24(5)6)30(7)27(32)25(23(3
InchiKey: GMVUOSTWEVTAAD-UHFFFAOYSA-N
Formula: C29H56N2O5
SMILES: CCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)C(C(C)C)N(C)C(=O)OCCCCCCCC
Mol. weight [g/mol]: 512.77

Physical Properties

Property code	Value	Unit	Source
gf	-191.66	kJ/mol	Joback Method
hf	-1130.13	kJ/mol	Joback Method
hfus	69.99	kJ/mol	Joback Method
hvap	107.74	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	6.827		Crippen Method
mcvol	455.880	ml/mol	McGowan Method
pc	685.65	kPa	Joback Method
rinpol	3089.00		NIST Webbook
tb	1092.49	K	Joback Method
tc	1371.32	K	Joback Method
tf	615.78	K	Joback Method
vc	1.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1647.65	J/mol×K	1092.49	Joback Method
cpg	1668.59	J/mol×K	1138.96	Joback Method
cpg	1686.98	J/mol×K	1185.43	Joback Method
cpg	1702.98	J/mol×K	1231.90	Joback Method
cpg	1716.74	J/mol×K	1278.38	Joback Method
cpg	1728.44	J/mol×K	1324.85	Joback Method
cpg	1738.24	J/mol×K	1371.32	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=U392911&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