

DL-Valine, N-methyl-N-(vinylloxycarbonyl)-, nonyl ester

Inchi:	InChI=1S/C18H33NO4/c1-6-8-9-10-11-12-13-14-23-17(20)16(15(3)4)19(5)18(21)22-7-2/
InchiKey:	FFRTZCNMZCICMS-UHFFFAOYSA-N
Formula:	C18H33NO4
SMILES:	C=COC(=O)N(C)C(C(=O)OCCCCCCCCC)C(C)C
Mol. weight [g/mol]:	327.46

Physical Properties

Property code	Value	Unit	Source
gf	-173.42	kJ/mol	Joback Method
hf	-722.05	kJ/mol	Joback Method
hfus	42.64	kJ/mol	Joback Method
hvap	74.57	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.517		Crippen Method
mcvol	285.040	ml/mol	McGowan Method
pc	1277.33	kPa	Joback Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tb	772.06	K	Joback Method
tc	954.99	K	Joback Method
tf	437.65	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.89	J/molxK	772.06	Joback Method
cpg	884.20	J/molxK	802.55	Joback Method
cpg	900.54	J/molxK	833.04	Joback Method
cpg	915.92	J/molxK	863.52	Joback Method
cpg	930.36	J/molxK	894.01	Joback Method
cpg	943.89	J/molxK	924.50	Joback Method
cpg	956.52	J/molxK	954.99	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=U393040&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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