DL-Valine, N-methyl-N-(but-3-yn-1-yloxycarbonyl)-, nonyl ester

Inchi: InChI=1S/C20H35NO4/c1-6-8-10-11-12-13-14-16-24-19(22)18(17(3)4)21(5)20(23)25-15-

InchiKey: KPKUMHHBWBRZMM-UHFFFAOYSA-N

Formula: C20H35NO4

SMILES: C#CCCOC(=O)N(C)C(C(=O)OCCCCCCCCC)C(C)C

Mol. weight [g/mol]: 353.50

Physical Properties

Property code	Value	Unit	Source
gf	-21.35	kJ/mol	Joback Method
hf	-596.86	kJ/mol	Joback Method
hfus	52.08	kJ/mol	Joback Method
hvap	79.55	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.397		Crippen Method
mcvol	308.920	ml/mol	McGowan Method
pc	1202.29	kPa	Joback Method
rinpol	2238.00		NIST Webbook
rinpol	2238.00		NIST Webbook
tb	811.26	K	Joback Method
tc	999.75	K	Joback Method
tf	508.92	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.49	J/mol×K	811.26	Joback Method
cpg	975.02	J/mol×K	842.68	Joback Method
cpg	991.50	J/mol×K	874.09	Joback Method
cpg	1006.96	J/mol×K	905.51	Joback Method
cpg	1021.43	J/mol×K	936.92	Joback Method
cpg	1034.94	J/mol×K	968.34	Joback Method
cpg	1047.51	J/mol×K	999.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392935&Units=SI
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

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

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