

DL-Valine, N-methyl-N-(but-3-yn-1-yloxy-carbonyl)-, undecyl ester

InChI: InChI=1S/C22H39NO4/c1-6-8-10-11-12-13-14-15-16-18-26-21(24)20(19(3)4)23(5)22(25)
InChIKey: MPPMKPJAYNBXGX-UHFFFAOYSA-N

Formula: C22H39NO4

SMILES: C#CCCCOC(=O)N(C)C(C(=O)OCCCCCCCCCCC)C(C)C

Mol. weight [g/mol]: 381.55

Physical Properties

Property code	Value	Unit	Source
gf	-4.51	kJ/mol	Joback Method
hf	-638.14	kJ/mol	Joback Method
hfus	57.26	kJ/mol	Joback Method
hvap	84.00	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.177		Crippen Method
mvol	337.100	ml/mol	McGowan Method
pc	1056.88	kPa	Joback Method
rinpol	2441.00		NIST Webbook
rinpol	2441.00		NIST Webbook
tb	857.02	K	Joback Method
tc	1050.84	K	Joback Method
tf	531.46	K	Joback Method
vc	1.284	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1078.76	J/mol×K	857.02	Joback Method
cpg	1096.96	J/mol×K	889.32	Joback Method
cpg	1114.01	J/mol×K	921.63	Joback Method
cpg	1129.94	J/mol×K	953.93	Joback Method
cpg	1144.79	J/mol×K	986.23	Joback Method
cpg	1158.58	J/mol×K	1018.53	Joback Method
cpg	1171.36	J/mol×K	1050.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U392937&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
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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