

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

InChI: InChI=1S/C23H41NO4/c1-6-8-10-11-12-13-14-15-16-17-19-27-22(25)21(20(3)4)24(5)23
InChIKey: REHHMRHQAMNRMG-UHFFFAOYSA-N

Formula: C23H41NO4

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

Mol. weight [g/mol]: 395.58

Physical Properties

Property code	Value	Unit	Source
gf	3.91	kJ/mol	Joback Method
hf	-658.78	kJ/mol	Joback Method
hfus	59.85	kJ/mol	Joback Method
hvap	86.23	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.567		Crippen Method
mvol	351.190	ml/mol	McGowan Method
pc	993.88	kPa	Joback Method
rinpol	2547.00		NIST Webbook
rinpol	2547.00		NIST Webbook
tb	879.90	K	Joback Method
tc	1077.60	K	Joback Method
tf	542.73	K	Joback Method
vc	1.339	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1140.44	J/molxK	879.90	Joback Method
cpg	1159.03	J/molxK	912.85	Joback Method
cpg	1176.38	J/molxK	945.80	Joback Method
cpg	1192.56	J/molxK	978.75	Joback Method
cpg	1207.59	J/molxK	1011.70	Joback Method
cpg	1221.52	J/molxK	1044.65	Joback Method
cpg	1234.39	J/molxK	1077.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392938&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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