DL-Alanine, N-methyl-N-(byt-3-yn-1-yloxycarbonyl)-, dodecyl ester

Inchi: InChI=1S/C21H37NO4/c1-5-7-9-10-11-12-13-14-15-16-18-25-20(23)19(3)22(4)21(24)26-
InchiKey: GWAXVRHHCYKOCO-UHFFFAOYSA-N
Formula: C21H37NO4
SMILES: C#CCCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCCC
Mol. weight [g/mol]: 367.52

Physical Properties

Property code	Value	Unit	Source
gf	-10.49	kJ/mol	Joback Method
hf	-612.22	kJ/mol	Joback Method
hfus	58.19	kJ/mol	Joback Method
hvap	82.17	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.931		Crippen Method
mcvol	323.010	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook
tb	834.58	K	Joback Method
tc	1024.52	K	Joback Method
tf	535.19	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.27	J/mol×K	834.58	Joback Method
cpg	1035.05	J/mol×K	866.24	Joback Method
cpg	1051.76	J/mol×K	897.89	Joback Method
cpg	1067.42	J/mol×K	929.55	Joback Method
cpg	1082.06	J/mol×K	961.21	Joback Method
cpg	1095.72	J/mol×K	992.86	Joback Method
cpg	1108.42	J/mol×K	1024.52	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=U392709&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
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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