

DL-Alanine, N-methyl-N-(but-3-yn-1-yloxy carbonyl)-, tridecyl ester

InChI: InChI=1S/C22H39NO4/c1-5-7-9-10-11-12-13-14-15-16-17-19-26-21(24)20(3)23(4)22(25)
InChIKey: KVONDWABJOVAPK-UHFFFAOYSA-N

Formula: C22H39NO4

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

Mol. weight [g/mol]: 381.55

Physical Properties

Property code	Value	Unit	Source
gf	-2.07	kJ/mol	Joback Method
hf	-632.86	kJ/mol	Joback Method
hfus	60.78	kJ/mol	Joback Method
hvap	84.39	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.321		Crippen Method
mvol	337.100	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	2510.00		NIST Webbook
rinpol	2510.00		NIST Webbook
tb	857.46	K	Joback Method
tc	1050.78	K	Joback Method
tf	546.46	K	Joback Method
vc	1.290	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1078.29	J/molxK	857.46	Joback Method
cpg	1096.46	J/molxK	889.68	Joback Method
cpg	1113.49	J/molxK	921.90	Joback Method
cpg	1129.41	J/molxK	954.12	Joback Method
cpg	1144.27	J/molxK	986.34	Joback Method
cpg	1158.09	J/molxK	1018.56	Joback Method
cpg	1170.92	J/molxK	1050.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392710&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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