

DL-Alanine, N-methyl-N-(but-2-yn-1-yloxy carbonyl)-, hexyl

InChI:
ester

InChI=1S/C15H25NO4/c1-5-7-9-10-12-19-14(17)13(3)16(4)15(18)20-11-8-6-2/h13H,5,7,

InChIKey:

XNFCPAALCITZOP-UHFFFAOYSA-N

Formula:

C15H25NO4

SMILES:

CC#CCOC(=O)N(C)C(C)C(=O)OCCCCC

Mol. weight [g/mol]:

283.36

Physical Properties

Property code	Value	Unit	Source
gf	-81.28	kJ/mol	Joback Method
hf	-507.98	kJ/mol	Joback Method
hfus	42.80	kJ/mol	Joback Method
hvap	71.10	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.590		Crippen Method
mvol	238.470	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	1947.00		NIST Webbook
rinpol	1947.00		NIST Webbook
tb	716.18	K	Joback Method
tc	907.34	K	Joback Method
tf	526.70	K	Joback Method
vc	0.897	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.51	J/molxK	716.18	Joback Method
cpg	689.47	J/molxK	748.04	Joback Method
cpg	704.55	J/molxK	779.90	Joback Method
cpg	718.77	J/molxK	811.76	Joback Method
cpg	732.13	J/molxK	843.62	Joback Method
cpg	744.65	J/molxK	875.48	Joback Method
cpg	756.33	J/molxK	907.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392717&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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