

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

InChI: InChI=1S/C12H19NO4/c1-5-7-9-17-12(15)13(4)10(3)11(14)16-8-6-2/h10H,6,8-9H2,1-4H3
InChIKey: AMSJCALWSRWSFA-UHFFFAOYSA-N

Formula: C12H19NO4

SMILES: CC#CCOC(=O)N(C)C(C)C(=O)OCCC

Mol. weight [g/mol]: 241.28

Physical Properties

Property code	Value	Unit	Source
gf	-106.54	kJ/mol	Joback Method
hf	-446.06	kJ/mol	Joback Method
hfus	35.03	kJ/mol	Joback Method
hvap	64.42	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.420		Crippen Method
mvol	196.200	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	1657.00		NIST Webbook
rinpol	1657.00		NIST Webbook
tb	647.54	K	Joback Method
tc	843.92	K	Joback Method
tf	492.89	K	Joback Method
vc	0.730	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.01	J/molxK	647.54	Joback Method
cpg	527.59	J/molxK	680.27	Joback Method
cpg	541.41	J/molxK	713.00	Joback Method
cpg	554.49	J/molxK	745.73	Joback Method
cpg	566.81	J/molxK	778.46	Joback Method
cpg	578.39	J/molxK	811.19	Joback Method
cpg	589.24	J/molxK	843.92	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=U392716&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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