

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

InChI: InChI=1S/C13H21NO4/c1-6-7-8-17-13(16)14(5)11(4)12(15)18-9-10(2)3/h1,10-11H,7-9H2
InChIKey: NFUACZCPMBGRIU-UHFFFAOYSA-N

Formula: C13H21NO4

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

Mol. weight [g/mol]: 255.31

Physical Properties

Property code	Value	Unit	Source
gf	-80.29	kJ/mol	Joback Method
hf	-452.38	kJ/mol	Joback Method
hfus	33.95	kJ/mol	Joback Method
hvap	63.97	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.666		Crippen Method
mvol	210.290	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
rinpol	1619.00		NIST Webbook
rinpol	1619.00		NIST Webbook
tb	651.10	K	Joback Method
tc	840.54	K	Joback Method
tf	430.03	K	Joback Method
vc	0.779	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.62	J/molxK	651.10	Joback Method
cpg	577.58	J/molxK	682.67	Joback Method
cpg	591.75	J/molxK	714.25	Joback Method
cpg	605.15	J/molxK	745.82	Joback Method
cpg	617.79	J/molxK	777.40	Joback Method
cpg	629.68	J/molxK	808.97	Joback Method
cpg	640.84	J/molxK	840.54	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=U392700&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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