

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

InChI:
ester

InChI=1S/C18H31NO4/c1-5-7-9-10-11-12-13-15-22-17(20)16(3)19(4)18(21)23-14-8-6-2/

InChIKey:

DMQRVYWDBPVVPL-UHFFFAOYSA-N

Formula:

C18H31NO4

SMILES:

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

Mol. weight [g/mol]:

325.44

Physical Properties

Property code	Value	Unit	Source
gf	-56.02	kJ/mol	Joback Method
hf	-569.90	kJ/mol	Joback Method
hfus	50.57	kJ/mol	Joback Method
hvap	77.78	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.760		Crippen Method
mvol	280.740	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	2203.00		NIST Webbook
rinpol	2203.00		NIST Webbook
tb	784.82	K	Joback Method
tc	975.05	K	Joback Method
tf	560.51	K	Joback Method
vc	1.065	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.49	J/molxK	784.82	Joback Method
cpg	861.43	J/molxK	816.52	Joback Method
cpg	877.38	J/molxK	848.23	Joback Method
cpg	892.35	J/molxK	879.93	Joback Method
cpg	906.35	J/molxK	911.64	Joback Method
cpg	919.41	J/molxK	943.34	Joback Method
cpg	931.54	J/molxK	975.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392721&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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