

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

Inchi:
ester

InChI=1S/C19H33NO4/c1-5-7-9-10-11-12-13-14-16-23-18(21)17(3)20(4)19(22)24-15-8-6

InchiKey:

KQLIOIXIELKITC-UHFFFAOYSA-N

Formula:

C19H33NO4

SMILES:

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

Mol. weight [g/mol]:

339.47

Physical Properties

Property code	Value	Unit	Source
gf	-47.60	kJ/mol	Joback Method
hf	-590.54	kJ/mol	Joback Method
hfus	53.16	kJ/mol	Joback Method
hvap	80.01	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.151		Crippen Method
mvol	294.830	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
tb	807.70	K	Joback Method
tc	998.80	K	Joback Method
tf	571.78	K	Joback Method
vc	1.121	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.42	J/molxK	807.70	Joback Method
cpg	920.66	J/molxK	839.55	Joback Method
cpg	936.85	J/molxK	871.40	Joback Method
cpg	952.03	J/molxK	903.25	Joback Method
cpg	966.19	J/molxK	935.10	Joback Method
cpg	979.38	J/molxK	966.95	Joback Method
cpg	991.60	J/molxK	998.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392722&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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