

DL-Alanine, N-methyl-N-(but-2-yn-1-yloxycarbonyl)-, octyl

InChI:
ester

InChI=1S/C17H29NO4/c1-5-7-9-10-11-12-14-21-16(19)15(3)18(4)17(20)22-13-8-6-2/h15

InChIKey:

UMBPROZFZBYJDN-UHFFFAOYSA-N

Formula:

C17H29NO4

SMILES:

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

Mol. weight [g/mol]:

311.42

Physical Properties

Property code	Value	Unit	Source
gf	-64.44	kJ/mol	Joback Method
hf	-549.26	kJ/mol	Joback Method
hfus	47.98	kJ/mol	Joback Method
hvap	75.56	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.370		Crippen Method
mvol	266.650	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	2120.00		NIST Webbook
rinpol	2120.00		NIST Webbook
tb	761.94	K	Joback Method
tc	951.92	K	Joback Method
tf	549.24	K	Joback Method
vc	1.010	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.47	J/mol×K	761.94	Joback Method
cpg	803.11	J/mol×K	793.60	Joback Method
cpg	818.80	J/mol×K	825.27	Joback Method
cpg	833.54	J/mol×K	856.93	Joback Method
cpg	847.36	J/mol×K	888.60	Joback Method
cpg	860.28	J/mol×K	920.26	Joback Method
cpg	872.29	J/mol×K	951.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392720&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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