

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

InChI: InChI=1S/C16H27NO4/c1-5-7-9-10-11-13-20-15(18)14(3)17(4)16(19)21-12-8-6-2/h14H,5
InChIKey: GQYHMYKIRNLMDG-UHFFFAOYSA-N

Formula: C16H27NO4

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

Mol. weight [g/mol]: 297.39

Physical Properties

Property code	Value	Unit	Source
gf	-72.86	kJ/mol	Joback Method
hf	-528.62	kJ/mol	Joback Method
hfus	45.39	kJ/mol	Joback Method
hvap	73.33	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.980		Crippen Method
mcvol	252.560	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rinpol	2033.00		NIST Webbook
rinpol	2033.00		NIST Webbook
tb	739.06	K	Joback Method
tc	929.37	K	Joback Method
tf	537.97	K	Joback Method
vc	0.954	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.45	J/mol×K	739.06	Joback Method
cpg	745.77	J/mol×K	770.78	Joback Method
cpg	761.17	J/mol×K	802.50	Joback Method
cpg	775.67	J/mol×K	834.22	Joback Method
cpg	789.28	J/mol×K	865.93	Joback Method
cpg	802.01	J/mol×K	897.65	Joback Method
cpg	813.88	J/mol×K	929.37	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=U392719&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
hvap:	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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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