D-Alanine, N-propargyloxycarbonyl-, isohexyl ester

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

InchiKey: AYVQOFBIFHCAHI-UHFFFAOYSA-N

Formula: C13H21NO4

SMILES: C#CCOC(=O)NC(C)C(=O)OCCCC(C)C

Mol. weight [g/mol]: 255.31

Physical Properties

Property code	Value	Unit	Source
gf	-101.68	kJ/mol	Joback Method
hf	-466.44	kJ/mol	Joback Method
hfus	36.03	kJ/mol	Joback Method
hvap	68.36	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	1.714		Crippen Method
mcvol	210.290	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpol	1725.00		NIST Webbook
rinpol	1725.00		NIST Webbook
tb	688.83	K	Joback Method
tc	881.46	K	Joback Method
tf	450.22	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.59	J/mol×K	688.83	Joback Method
cpg	592.91	J/mol×K	720.94	Joback Method
cpg	606.46	J/mol×K	753.04	Joback Method
cpg	619.22	J/mol×K	785.15	Joback Method
cpg	631.22	J/mol×K	817.25	Joback Method
cpg	642.46	J/mol×K	849.36	Joback Method
cpg	652.95	J/mol×K	881.46	Joback Method

Sources

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=U347741&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume