D-Alanine, N-propargyloxycarbonyl-, decyl ester

Inchi: InChI=1S/C17H29NO4/c1-4-6-7-8-9-10-11-12-14-21-16(19)15(3)18-17(20)22-13-5-2/h2,1

InchiKey: XLFRZGAAUMANDM-UHFFFAOYSA-N

Formula: C17H29NO4

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

Mol. weight [g/mol]: 311.42

Physical Properties

Property code	Value	Unit	Source
gf	-65.56	kJ/mol	Joback Method
hf	-543.72	kJ/mol	Joback Method
hfus	49.91	kJ/mol	Joback Method
hvap	77.65	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.418		Crippen Method
mcvol	266.650	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	2149.00		NIST Webbook
rinpol	2149.00		NIST Webbook
tb	780.79	K	Joback Method
tc	969.01	K	Joback Method
tf	510.30	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.85	J/mol×K	780.79	Joback Method
cpg	815.57	J/mol×K	812.16	Joback Method
cpg	830.38	J/mol×K	843.53	Joback Method
cpg	844.29	J/mol×K	874.90	Joback Method
cpg	857.32	J/mol×K	906.27	Joback Method
cpg	869.49	J/mol×K	937.64	Joback Method
cpg	880.80	J/mol×K	969.01	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=U347742&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