D-Alanine, N-propargyloxycarbonyl-, dodecyl ester

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

InchiKey: PRUPDCAVCBPHCS-UHFFFAOYSA-N

Formula: C19H33NO4

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

Mol. weight [g/mol]: 339.47

Physical Properties

Property code	Value	Unit	Source
gf	-48.72	kJ/mol	Joback Method
hf	-585.00	kJ/mol	Joback Method
hfus	55.09	kJ/mol	Joback Method
hvap	82.11	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.198		Crippen Method
mcvol	294.830	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinpol	2337.00		NIST Webbook
tb	826.55	K	Joback Method
tc	1017.57	K	Joback Method
tf	532.84	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.82	J/mol×K	826.55	Joback Method
cpg	933.24	J/mol×K	858.39	Joback Method
cpg	948.66	J/mol×K	890.22	Joback Method
cpg	963.08	J/mol×K	922.06	Joback Method
cpg	976.53	J/mol×K	953.90	Joback Method
cpg	989.04	J/mol×K	985.73	Joback Method
cpg	1000.62	J/mol×K	1017.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347743&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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