D-Alanine, N-allyloxycarbonyl-, undecyl ester

Inchi: InChI=1S/C18H33NO4/c1-4-6-7-8-9-10-11-12-13-15-22-17(20)16(3)19-18(21)23-14-5-2/h
InchiKey: OVJFYNCZIOCSJK-UHFFFAOYSA-N
Formula: C18H33NO4
SMILES: C=CCOC(O)=NC(C)C(=O)OCCCCCCCCCCC
Mol. weight [g/mol]: 327.46

Physical Properties

Property code	Value	Unit	Source
hf	-751.52	kJ/mol	Joback Method
hvap	86.24	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.566		Crippen Method
mcvol	285.040	ml/mol	McGowan Method
pc	1209.83	kPa	Joback Method
rinpol	2221.00		NIST Webbook
rinpol	2221.00		NIST Webbook
tb	874.93	K	Joback Method
tc	1071.85	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U347734&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

hf: Enthalpy of formation 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