«beta»-Alanine, N-allyloxycarbonyl-, decyl ester

Inchi: InChI=1S/C17H31NO4/c1-3-5-6-7-8-9-10-11-15-21-16(19)12-13-18-17(20)22-14-4-2/h4H

InchiKey: SSETYSXJFCTLGT-UHFFFAOYSA-N

Formula: C17H31NO4

SMILES: C=CCOC(O)=NCCC(=O)OCCCCCCCCCC

Mol. weight [g/mol]: 313.43

Physical Properties

Property code	Value	Unit	Source
hf	-725.60	kJ/mol	Joback Method
hvap	84.41	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	4.177		Crippen Method
mcvol	270.950	ml/mol	McGowan Method
pc	1287.44	kPa	Joback Method
rinpol	2258.00		NIST Webbook
tb	852.49	K	Joback Method
tc	1045.21	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321038&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

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