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

Inchi: InChI=1S/C19H35NO4/c1-3-5-6-7-8-9-10-11-12-13-17-23-18(21)14-15-20-19(22)24-16-4

InchiKey: LNROTORHUHAEEZ-UHFFFAOYSA-N

Formula: C19H35NO4

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

Mol. weight [g/mol]: 341.49

Physical Properties

Property code	Value	Unit	Source
hf	-766.88	kJ/mol	Joback Method
hvap	88.86	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.957		Crippen Method
mcvol	299.130	ml/mol	McGowan Method
pc	1126.83	kPa	Joback Method
rinpol	2464.00		NIST Webbook
rinpol	2464.00		NIST Webbook
tb	898.25	K	Joback Method
tc	1099.72	K	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=U321040&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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