DL-3-Aminobutanoic acid, N-hexyloxycarbonyl-, decyl ester

Inchi: InChI=1S/C21H41NO4/c1-4-6-8-10-11-12-13-15-16-25-20(23)18-19(3)22-21(24)26-17-14

InchiKey: YIILVZHDHKITPV-UHFFFAOYSA-N

Formula: C21H41NO4

SMILES: CCCCCCCCCCOC(=O)CC(C)N=C(O)OCCCCCC

Mol. weight [g/mol]: 371.55

Physical Properties

Property code	Value	Unit	Source
hf	-938.87	kJ/mol	Joback Method
hvap	93.59	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	5.960		Crippen Method
mcvol	331.610	ml/mol	McGowan Method
pc	973.52	kPa	Joback Method
rinpol	2503.00		NIST Webbook
rinpol	2503.00		NIST Webbook
tb	946.89	K	Joback Method
tc	1161.84	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=U392812&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