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

Inchi: InChI=1S/C25H49NO4/c1-4-6-8-10-11-12-13-14-15-16-17-19-20-29-24(27)22-23(3)26-25

InchiKey: QXMFHWOCNDKWDA-UHFFFAOYSA-N

Formula: C25H49NO4

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

Mol. weight [g/mol]: 427.66

Physical Properties

Property code	Value	Unit	Source
hf	-1021.43	kJ/mol	Joback Method
hvap	102.49	kJ/mol	Joback Method
log10ws	-7.83		Crippen Method
logp	7.520		Crippen Method
mcvol	387.970	ml/mol	McGowan Method
pc	776.34	kPa	Joback Method
rinpol	2882.00		NIST Webbook
rinpol	2882.00		NIST Webbook
tb	1038.41	K	Joback Method
tc	1293.43	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392815&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