l-Norvaline, n-butoxycarbonyl-, tetradecyl ester

Inchi: InChI=1S/C24H47NO4/c1-4-7-9-10-11-12-13-14-15-16-17-18-21-28-23(26)22(19-6-3)25-

InchiKey: ZMMTYOUQQZBHTJ-UHFFFAOYSA-N

Formula: C24H47NO4

SMILES: CCCCCCCCCCCCCCOC(=O)C(CCC)N=C(O)OCCCC

Mol. weight [g/mol]: 413.63

Physical Properties

Property code	Value	Unit	Source
hf	-1000.79	kJ/mol	Joback Method
hvap	100.27	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	7.130		Crippen Method
mcvol	373.880	ml/mol	McGowan Method
pc	819.60	kPa	Joback Method
tb	1015.53	K	Joback Method
tc	1258.49	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320780&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature