l-Norvaline, n-butoxycarbonyl-, heptadecyl ester

Inchi: InChI=1S/C27H53NO4/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-21-24-31-26(29)25(2

InchiKey: FHKDLCAPWXZGSG-UHFFFAOYSA-N

Formula: C27H53NO4

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

Mol. weight [g/mol]: 455.71

Physical Properties

Property code	Value	Unit	Source
hf	-1062.71	kJ/mol	Joback Method
hvap	106.95	kJ/mol	Joback Method
log10ws	-8.66		Crippen Method
logp	8.300		Crippen Method
mcvol	416.150	ml/mol	McGowan Method
pc	699.50	kPa	Joback Method
tb	1084.17	K	Joback Method
tc	1368.09	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320783&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature