L-Norvaline, N-octyloxycarbonyl-, dodecyl ester

Inchi: InChI=1S/C26H51NO4/c1-4-7-9-11-13-14-15-16-18-19-22-30-25(28)24(21-6-3)27-26(29)

InchiKey: OQMXQSZICIIMCH-XMMPIXPASA-N

Formula: C26H51NO4

SMILES: CCCCCCCCCCCCOC(=O)C(CCC)N=C(O)OCCCCCCCC

Mol. weight [g/mol]: 441.69

Physical Properties

Property code	Value	Unit	Source
hf	-1042.07	kJ/mol	Joback Method
hvap	104.72	kJ/mol	Joback Method
log10ws	-8.25		Crippen Method
logp	7.910		Crippen Method
mcvol	402.060	ml/mol	McGowan Method
pc	736.42	kPa	Joback Method
rinpol	2985.00		NIST Webbook
rinpol	2985.00		NIST Webbook
tb	1061.29	K	Joback Method
tc	1329.92	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392852&Units=SI

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