L-Norvaline, N-octyloxycarbonyl-, undecyl ester

Inchi: InChI=1S/C25H49NO4/c1-4-7-9-11-13-14-15-17-18-21-29-24(27)23(20-6-3)26-25(28)30-

InchiKey: KJLICIPCZAOWEQ-HSZRJFAPSA-N

Formula: C25H49NO4

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

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	2886.00		NIST Webbook
rinpol	2886.00		NIST Webbook
tb	1038.41	K	Joback Method
tc	1293.43	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=U392851&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