L-Norvaline, N-allyloxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C15H27NO4/c1-5-8-13(16-15(18)20-10-6-2)14(17)19-11-7-9-12(3)4/h6,12-13H

InchiKey: JISMMAQOALHKMT-UHFFFAOYSA-N

Formula: C15H27NO4

SMILES: C=CCOC(=O)NC(CCC)C(=O)OCCCC(C)C

Mol. weight [g/mol]: 285.38

Physical Properties

Property code	Value	Unit	Source
hfus	36.95	kJ/mol	Joback Method
logp	3.047		Crippen Method
mcvol	242.770	ml/mol	McGowan Method
rinpol	1709.00		NIST Webbook
rinpol	1709.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.24	J/mol×K	741.15	Joback Method
cpg	728.85	J/mol×K	772.08	Joback Method
cpg	743.58	J/mol×K	803.02	Joback Method
cpg	757.46	J/mol×K	833.95	Joback Method
cpg	770.48	J/mol×K	864.89	Joback Method
cpg	782.66	J/mol×K	895.82	Joback Method
cpg	794.02	J/mol×K	926.76	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320746&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices