L-Norvaline, N-isobutoxycarbonyl-, pentyl ester

Inchi: InChI=1S/C15H29NO4/c1-5-7-8-10-19-14(17)13(9-6-2)16-15(18)20-11-12(3)4/h12-13H,5

InchiKey: QQLUMINGEMLSLV-UHFFFAOYSA-N

Formula: C15H29NO4

SMILES: CCCCCOC(=O)C(CCC)NC(=O)OCC(C)C

Mol. weight [g/mol]: 287.40

Physical Properties

Property code	Value	Unit	Source
hf	-986.75	kJ/mol	Cheméo Relay (1.0)
hfus	38.23	kJ/mol	Joback Method
hvap	83.43	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.80		Cheméo Relay (1.0)
logp	3.271		Crippen Method
mcvol	247.070	ml/mol	McGowan Method
rinpol	1706.00		NIST Webbook
tb	571.42	K	Cheméo Relay (1.0)
tf	275.69	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.37	J/mol×K	744.47	Joback Method
cpg	754.49	J/mol×K	775.11	Joback Method
cpg	769.73	J/mol×K	805.76	Joback Method
cpg	784.09	J/mol×K	836.40	Joback Method
cpg	797.58	J/mol×K	867.04	Joback Method
cpg	810.20	J/mol×K	897.69	Joback Method
cpg	821.97	J/mol×K	928.33	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=U320715&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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point