l-Norvaline, n-butoxycarbonyl-, ethyl ester

Inchi: InChI=1S/C12H23NO4/c1-4-7-9-17-12(15)13-10(8-5-2)11(14)16-6-3/h10H,4-9H2,1-3H3,(
InchiKey: NLKNCZZOOBSECJ-UHFFFAOYSA-N
Formula: C12H23NO4
SMILES: CCCCOC(O)=NC(CCC)C(=O)OCC
Mol. weight [g/mol]: 245.32

Physical Properties

Property code	Value	Unit	Source
hf	-753.11	kJ/mol	Joback Method
hvap	73.56	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.449		Crippen Method
mcvol	204.800	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
rinpol	1536.00		NIST Webbook
rinpol	1536.00		NIST Webbook
tb	740.97	K	Joback Method
tc	925.58	K	Joback Method

Sources

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=U320769&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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