l-Norvaline, N-isobutoxycarbonyl-, ethyl ester

Inchi: InChI=1S/C12H23NO4/c1-5-7-10(11(14)16-6-2)13-12(15)17-8-9(3)4/h9-10H,5-8H2,1-4H
InchiKey: DCSNJOIXNSTESP-UHFFFAOYSA-N
Formula: C12H23NO4
SMILES: CCCC(NC(=O)OCC(C)C)C(=O)OCC
Mol. weight [g/mol]: 245.32

Physical Properties

Property code	Value	Unit	Source
gf	-333.17	kJ/mol	Joback Method
hf	-737.70	kJ/mol	Joback Method
hfus	30.46	kJ/mol	Joback Method
hvap	66.28	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.100		Crippen Method
mcvol	204.800	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	1492.00		NIST Webbook
tb	675.83	K	Joback Method
tc	861.03	K	Joback Method
tf	391.98	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.60	J/mol×K	675.83	Joback Method
cpg	587.47	J/mol×K	706.70	Joback Method
cpg	601.58	J/mol×K	737.56	Joback Method
cpg	614.95	J/mol×K	768.43	Joback Method
cpg	627.56	J/mol×K	799.30	Joback Method
cpg	639.42	J/mol×K	830.16	Joback Method
cpg	650.54	J/mol×K	861.03	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=U320712&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume