l-Leucine, N-isobutoxycarbonyl-N-methyl-, propyl ester

Inchi: InChI=1S/C15H29NO4/c1-7-8-19-14(17)13(9-11(2)3)16(6)15(18)20-10-12(4)5/h11-13H,7

InchiKey: XDDHAEQAZYGRQX-UHFFFAOYSA-N

Formula: C15H29NO4

SMILES: CCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(C)C

Mol. weight [g/mol]: 287.40

Physical Properties

Property code	Value	Unit	Source
gf	-288.96	kJ/mol	Joback Method
hf	-790.84	kJ/mol	Joback Method
hfus	32.63	kJ/mol	Joback Method
hvap	68.17	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	3.079		Crippen Method
mcvol	247.070	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	1699.00		NIST Webbook
rinpol	1699.00		NIST Webbook
tb	706.30	K	Joback Method
tc	888.08	K	Joback Method
tf	390.60	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.52	J/mol×K	706.30	Joback Method
cpg	736.51	J/mol×K	736.60	Joback Method
cpg	752.61	J/mol×K	766.89	Joback Method
cpg	767.83	J/mol×K	797.19	Joback Method
cpg	782.17	J/mol×K	827.48	Joback Method
cpg	795.66	J/mol×K	857.78	Joback Method
cpg	808.30	J/mol×K	888.08	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=U321868&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