l-Leucine, N-methyl-n-propoxycarbonyl-, butyl ester

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

InchiKey: MGQQLIZADNXVLK-UHFFFAOYSA-N

Formula: C15H29NO4

SMILES: CCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCC

Mol. weight [g/mol]: 287.40

Physical Properties

Property code	Value	Unit	Source
gf	-286.52	kJ/mol	Joback Method
hf	-785.56	kJ/mol	Joback Method
hfus	36.15	kJ/mol	Joback Method
hvap	68.56	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.223		Crippen Method
mcvol	247.070	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpol	1732.00		NIST Webbook
rinpol	1732.00		NIST Webbook
tb	706.74	K	Joback Method
tc	886.30	K	Joback Method
tf	405.60	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.05	J/mol×K	706.74	Joback Method
cpg	735.81	J/mol×K	736.67	Joback Method
cpg	751.71	J/mol×K	766.59	Joback Method
cpg	766.75	J/mol×K	796.52	Joback Method
cpg	780.95	J/mol×K	826.45	Joback Method
cpg	794.33	J/mol×K	856.38	Joback Method
cpg	806.88	J/mol×K	886.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321855&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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