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

Inchi: InChI=1S/C16H31NO4/c1-6-8-10-20-15(18)14(12-13(3)4)17(5)16(19)21-11-9-7-2/h13-14
InchiKey: OGWAHWBCOSKDJB-UHFFFAOYSA-N
Formula: C16H31NO4
SMILES: CCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCCC
Mol. weight [g/mol]: 301.42

Physical Properties

Property code	Value	Unit	Source
gf	-278.10	kJ/mol	Joback Method
hf	-806.20	kJ/mol	Joback Method
hfus	38.74	kJ/mol	Joback Method
hvap	70.79	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.613		Crippen Method
mcvol	261.160	ml/mol	McGowan Method
pc	1426.15	kPa	Joback Method
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook
tb	729.62	K	Joback Method
tc	909.40	K	Joback Method
tf	416.87	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.01	J/mol×K	729.62	Joback Method
cpg	793.14	J/mol×K	759.58	Joback Method
cpg	809.36	J/mol×K	789.55	Joback Method
cpg	824.69	J/mol×K	819.51	Joback Method
cpg	839.14	J/mol×K	849.47	Joback Method
cpg	852.73	J/mol×K	879.44	Joback Method
cpg	865.46	J/mol×K	909.40	Joback Method

Sources

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=U321883&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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