L-leucine, n-butoxycarbonyl-n-methyl-, heptyl ester

Inchi: InChI=1S/C19H37NO4/c1-6-8-10-11-12-14-23-18(21)17(15-16(3)4)20(5)19(22)24-13-9-7

InchiKey: KQDYDDHSENQHLY-UHFFFAOYSA-N

Formula: C19H37NO4

SMILES: CCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCCC

Mol. weight [g/mol]: 343.51

Physical Properties

Property code	Value	Unit	Source
hf	-1011.41	kJ/mol	Cheméo Relay (1.0)
hfus	46.52	kJ/mol	Joback Method
hvap	94.38	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.40		Cheméo Relay (1.0)
logp	4.783		Crippen Method
mcvol	303.430	ml/mol	McGowan Method
rinpol	2101.00		NIST Webbook
tb	603.27	K	Cheméo Relay (1.0)
tf	245.01	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.86	J/mol×K	798.26	Joback Method
cpg	971.04	J/mol×K	828.91	Joback Method
cpg	988.16	J/mol×K	859.56	Joback Method
cpg	1004.24	J/mol×K	890.22	Joback Method
cpg	1019.32	J/mol×K	920.87	Joback Method
cpg	1033.40	J/mol×K	951.52	Joback Method
cpg	1046.51	J/mol×K	982.17	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321886&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point