L-Leucine, N-isobutoxycarbonyl-N-methyl-, heptyl ester

Inchi: InChI=1S/C19H37NO4/c1-7-8-9-10-11-12-23-18(21)17(13-15(2)3)20(6)19(22)24-14-16(4

InchiKey: ACKYEAJGFNRLEM-UHFFFAOYSA-N

Formula: C19H37NO4

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

Mol. weight [g/mol]: 343.51

Physical Properties

Property code	Value	Unit	Source
hf	-1028.76	kJ/mol	Cheméo Relay (1.0)
hfus	42.99	kJ/mol	Joback Method
hvap	90.79	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.47		Cheméo Relay (1.0)
logp	4.639		Crippen Method
mcvol	303.430	ml/mol	McGowan Method
rinpol	2058.00		NIST Webbook
rinpol	2058.00		NIST Webbook
tb	603.62	K	Cheméo Relay (1.0)
tf	253.31	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.34	J/mol×K	797.82	Joback Method
cpg	971.63	J/mol×K	828.65	Joback Method
cpg	988.84	J/mol×K	859.49	Joback Method
cpg	1005.00	J/mol×K	890.32	Joback Method
cpg	1020.12	J/mol×K	921.15	Joback Method
cpg	1034.23	J/mol×K	951.99	Joback Method
cpg	1047.35	J/mol×K	982.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321873&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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