L-Leucine, N-benzyloxycarbonyl-N-methyl-, butyl ester

Inchi: InChI=1S/C19H29NO4/c1-5-6-12-23-18(21)17(13-15(2)3)20(4)19(22)24-14-16-10-8-7-9-
InchiKey: MCKNSDLNKOPESH-UHFFFAOYSA-N
Formula: C19H29NO4
SMILES: CCCCOC(=O)C(CC(C)C)N(C)C(=O)OCc1ccccc1
Mol. weight [g/mol]: 335.44

Physical Properties

Property code	Value	Unit	Source
af	0.8320		Cheméo Relay (1.0)
hfus	40.56	kJ/mol	Joback Method
log10ws	-3.78		Cheméo Relay (1.0)
logp	4.013		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
pc	1473.62	kPa	Joback Method
rinpol	2192.00		NIST Webbook
tb	620.60	K	Cheméo Relay (1.0)
tc	825.57	K	Cheméo Relay (1.0)
tf	264.24	K	Cheméo Relay (1.0)
vc	1.009	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.81	J/mol×K	824.94	Joback Method
cpg	879.13	J/mol×K	858.65	Joback Method
cpg	894.27	J/mol×K	892.35	Joback Method
cpg	908.28	J/mol×K	926.06	Joback Method
cpg	921.18	J/mol×K	959.76	Joback Method
cpg	933.00	J/mol×K	993.47	Joback Method
cpg	943.80	J/mol×K	1027.17	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322037&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):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion 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