L-leucine, n-benzyloxycarbonyl-n-methyl-, undecyl ester

Inchi: InChI=1S/C26H43NO4/c1-5-6-7-8-9-10-11-12-16-19-30-25(28)24(20-22(2)3)27(4)26(29)

InchiKey: RBZRXDRYXUGKON-UHFFFAOYSA-N

Formula: C26H43NO4

SMILES: CCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCc1ccccc1

Mol. weight [g/mol]: 433.63

Physical Properties

Property code	Value	Unit	Source
hfus	58.69	kJ/mol	Joback Method
log10ws	-6.16		Cheméo Relay (1.0)
logp	6.744		Crippen Method
mcvol	378.300	ml/mol	McGowan Method
pc	931.21	kPa	Joback Method
rinpol	2907.00		NIST Webbook
tb	671.06	K	Cheméo Relay (1.0)
tf	285.92	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1288.99	J/mol×K	985.10	Joback Method
cpg	1306.64	J/mol×K	1021.98	Joback Method
cpg	1322.75	J/mol×K	1058.86	Joback Method
cpg	1337.38	J/mol×K	1095.74	Joback Method
cpg	1350.60	J/mol×K	1132.62	Joback Method
cpg	1362.49	J/mol×K	1169.50	Joback Method
cpg	1373.10	J/mol×K	1206.38	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322042&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
tf:	Normal melting (fusion) point