L-leucine, n-allyloxycarbonyl-n-methyl-, dodecyl ester

Inchi: InChI=1S/C23H43NO4/c1-6-8-9-10-11-12-13-14-15-16-18-27-22(25)21(19-20(3)4)24(5)2

InchiKey: VIFJAVGJSPVRCE-UHFFFAOYSA-N

Formula: C23H43NO4

SMILES: C=CCOC(=O)N(C)C(CC(C)C)C(=O)OCCCCCCCCCCCC

Mol. weight [g/mol]: 397.60

Physical Properties

Property code	Value	Unit	Source
hfus	55.60	kJ/mol	Joback Method
log10ws	-5.60		Cheméo Relay (1.0)
logp	6.120		Crippen Method
mcvol	355.490	ml/mol	McGowan Method
rinpol	2497.00		NIST Webbook
rinpol	2497.00		NIST Webbook
tb	651.19	K	Cheméo Relay (1.0)
tf	269.09	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1171.10	J/mol×K	886.46	Joback Method
cpg	1190.29	J/mol×K	919.60	Joback Method
cpg	1208.19	J/mol×K	952.74	Joback Method
cpg	1224.83	J/mol×K	985.87	Joback Method
cpg	1240.26	J/mol×K	1019.01	Joback Method
cpg	1254.52	J/mol×K	1052.15	Joback Method
cpg	1267.65	J/mol×K	1085.29	Joback Method

Sources

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=U321905&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point