L-Leucine, N-neopentyloxycarbonyl-N-methyl-, undecyl ester

Inchi: InChI=1S/C24H47NO4/c1-8-9-10-11-12-13-14-15-16-17-28-22(26)21(18-20(2)3)25(7)23(
InchiKey: UDTWLNOOKOZOKH-UHFFFAOYSA-N
Formula: C24H47NO4
SMILES: CCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]: 413.64

Physical Properties

Property code	Value	Unit	Source
hfus	52.05	kJ/mol	Joback Method
log10ws	-6.21		Cheméo Relay (1.0)
logp	6.590		Crippen Method
mcvol	373.880	ml/mol	McGowan Method
rinpol	2480.00		NIST Webbook
rinpol	2480.00		NIST Webbook
tb	635.33	K	Cheméo Relay (1.0)
tf	297.76	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1263.00	J/mol×K	909.43	Joback Method
cpg	1282.95	J/mol×K	943.44	Joback Method
cpg	1301.53	J/mol×K	977.46	Joback Method
cpg	1318.80	J/mol×K	1011.47	Joback Method
cpg	1334.83	J/mol×K	1045.48	Joback Method
cpg	1349.67	J/mol×K	1079.49	Joback Method
cpg	1363.38	J/mol×K	1113.51	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=U321914&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point