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]: 413.63

Physical Properties

Property code	Value	Unit	Source
gf	-207.90	kJ/mol	Joback Method
hf	-980.07	kJ/mol	Joback Method
hfus	52.05	kJ/mol	Joback Method
hvap	87.30	kJ/mol	Joback Method
log10ws	-6.77		Crippen Method
logp	6.590		Crippen Method
mcvol	373.880	ml/mol	McGowan Method
pc	866.58	kPa	Joback Method
rinpol	2480.00		NIST Webbook
rinpol	2480.00		NIST Webbook
tb	909.43	K	Joback Method
tc	1113.51	K	Joback Method
tf	509.45	K	Joback Method
vc	1.423	m3/kmol	Joback Method

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321914&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume