l-Leucine, N-neopentyloxycarbonyl-N-methyl-, dodecyl ester

Inchi: InChI=1S/C25H49NO4/c1-8-9-10-11-12-13-14-15-16-17-18-29-23(27)22(19-21(2)3)26(7)
InchiKey: LROMTVODLFAPTH-UHFFFAOYSA-N
Formula: C25H49NO4
SMILES: CCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]: 427.66

Physical Properties

Property code	Value	Unit	Source
gf	-199.48	kJ/mol	Joback Method
hf	-1000.71	kJ/mol	Joback Method
hfus	54.64	kJ/mol	Joback Method
hvap	89.53	kJ/mol	Joback Method
log10ws	-7.19		Crippen Method
logp	6.980		Crippen Method
mcvol	387.970	ml/mol	McGowan Method
pc	819.60	kPa	Joback Method
rinpol	2574.00		NIST Webbook
rinpol	2574.00		NIST Webbook
tb	932.31	K	Joback Method
tc	1142.50	K	Joback Method
tf	520.72	K	Joback Method
vc	1.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1326.59	J/mol×K	932.31	Joback Method
cpg	1347.00	J/mol×K	967.34	Joback Method
cpg	1365.95	J/mol×K	1002.37	Joback Method
cpg	1383.52	J/mol×K	1037.40	Joback Method
cpg	1399.77	J/mol×K	1072.44	Joback Method
cpg	1414.77	J/mol×K	1107.47	Joback Method
cpg	1428.59	J/mol×K	1142.50	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321915&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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