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

Inchi: InChI=1S/C28H55NO4/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21-32-26(30)25(22-24

InchiKey: GAVPSZMEXLQUAX-UHFFFAOYSA-N

Formula: C28H55NO4

SMILES: CCCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(C)(C)C

Mol. weight [g/mol]: 469.74

Physical Properties

Property code	Value	Unit	Source
gf	-174.22	kJ/mol	Joback Method
hf	-1062.63	kJ/mol	Joback Method
hfus	62.41	kJ/mol	Joback Method
hvap	96.21	kJ/mol	Joback Method
log10ws	-8.44		Crippen Method
logp	8.150		Crippen Method
mcvol	430.240	ml/mol	McGowan Method
pc	699.50	kPa	Joback Method
tb	1000.95	K	Joback Method
tc	1236.28	K	Joback Method
tf	554.53	K	Joback Method
vc	1.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.05	J/mol×K	1000.95	Joback Method
cpg	1542.17	J/mol×K	1040.17	Joback Method
cpg	1562.50	J/mol×K	1079.39	Joback Method
cpg	1581.13	J/mol×K	1118.61	Joback Method
cpg	1598.17	J/mol×K	1157.83	Joback Method
cpg	1613.74	J/mol×K	1197.06	Joback Method
cpg	1627.94	J/mol×K	1236.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321916&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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