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

Inchi: InChI=1S/C29H57NO4/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-33-27(31)26(23

InchiKey: PVWQLUUOXRDJGW-UHFFFAOYSA-N

Formula: C29H57NO4

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

Mol. weight [g/mol]: 483.77

Physical Properties

Property code	Value	Unit	Source
gf	-165.80	kJ/mol	Joback Method
hf	-1083.27	kJ/mol	Joback Method
hfus	65.00	kJ/mol	Joback Method
hvap	98.43	kJ/mol	Joback Method
log10ws	-8.86		Crippen Method
logp	8.540		Crippen Method
mcvol	444.330	ml/mol	McGowan Method
pc	665.29	kPa	Joback Method
rinpol	3078.00		NIST Webbook
rinpol	3078.00		NIST Webbook
tb	1023.83	K	Joback Method
tc	1270.11	K	Joback Method
tf	565.80	K	Joback Method
vc	1.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1585.28	J/mol×K	1023.83	Joback Method
cpg	1608.12	J/mol×K	1064.88	Joback Method
cpg	1628.99	J/mol×K	1105.92	Joback Method
cpg	1648.04	J/mol×K	1146.97	Joback Method
cpg	1665.40	J/mol×K	1188.02	Joback Method
cpg	1681.19	J/mol×K	1229.07	Joback Method
cpg	1695.55	J/mol×K	1270.11	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321917&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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