l-Leucine, N-methyl-n-propoxycarbonyl-, pentadecyl ester

Inchi: InChI=1S/C26H51NO4/c1-6-8-9-10-11-12-13-14-15-16-17-18-19-21-30-25(28)24(22-23(3

InchiKey: WECHBPNMDFVLJF-UHFFFAOYSA-N

Formula: C26H51NO4

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

Mol. weight [g/mol]: 441.69

Physical Properties

Property code	Value	Unit	Source
gf	-193.90	kJ/mol	Joback Method
hf	-1012.60	kJ/mol	Joback Method
hfus	64.65	kJ/mol	Joback Method
hvap	93.05	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	7.514		Crippen Method
mcvol	402.060	ml/mol	McGowan Method
pc	768.19	kPa	Joback Method
rinpol	2808.00		NIST Webbook
rinpol	2808.00		NIST Webbook
tb	958.42	K	Joback Method
tc	1180.17	K	Joback Method
tf	529.57	K	Joback Method
vc	1.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1390.97	J/mol×K	958.42	Joback Method
cpg	1412.29	J/mol×K	995.38	Joback Method
cpg	1431.89	J/mol×K	1032.34	Joback Method
cpg	1449.83	J/mol×K	1069.30	Joback Method
cpg	1466.16	J/mol×K	1106.26	Joback Method
cpg	1480.95	J/mol×K	1143.22	Joback Method
cpg	1494.27	J/mol×K	1180.17	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=U321864&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