L-Leucine, N-ethoxycarbonyl-N-methyl-, dodecyl ester

Inchi: InChI=1S/C22H43NO4/c1-6-8-9-10-11-12-13-14-15-16-17-27-21(24)20(18-19(3)4)23(5)2
InchiKey: KNOLYYLHJPWBSY-UHFFFAOYSA-N
Formula: C22H43NO4
SMILES: CCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC
Mol. weight [g/mol]: 385.59

Physical Properties

Property code	Value	Unit	Source
hf	-1075.52	kJ/mol	Cheméo Relay (1.0)
hfus	54.28	kJ/mol	Joback Method
hvap	110.08	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.53		Cheméo Relay (1.0)
logp	5.954		Crippen Method
mcvol	345.700	ml/mol	McGowan Method
rinpol	2419.00		NIST Webbook
rinpol	2419.00		NIST Webbook
tb	625.70	K	Cheméo Relay (1.0)
tf	272.60	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1137.05	J/mol×K	866.90	Joback Method
cpg	1156.38	J/mol×K	899.32	Joback Method
cpg	1174.44	J/mol×K	931.73	Joback Method
cpg	1191.26	J/mol×K	964.15	Joback Method
cpg	1206.88	J/mol×K	996.56	Joback Method
cpg	1221.34	J/mol×K	1028.98	Joback Method
cpg	1234.66	J/mol×K	1061.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321927&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point