l-Leucine, N-pivaloyl-, methyl ester

Inchi: InChI=1S/C12H23NO3/c1-8(2)7-9(10(14)16-6)13-11(15)12(3,4)5/h8-9H,7H2,1-6H3,(H,13
InchiKey: MCDZFMUYBNTHSQ-UHFFFAOYSA-N
Formula: C12H23NO3
SMILES: COC(=O)C(CC(C)C)NC(=O)C(C)(C)C
Mol. weight [g/mol]: 229.32

Physical Properties

Property code	Value	Unit	Source
gf	-225.33	kJ/mol	Joback Method
hf	-614.23	kJ/mol	Joback Method
hfus	21.86	kJ/mol	Joback Method
hvap	62.57	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.736		Crippen Method
mcvol	198.930	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	1405.00		NIST Webbook
tb	650.18	K	Joback Method
tc	844.80	K	Joback Method
tf	372.17	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.88	J/mol×K	650.18	Joback Method
cpg	563.53	J/mol×K	682.62	Joback Method
cpg	578.29	J/mol×K	715.05	Joback Method
cpg	592.20	J/mol×K	747.49	Joback Method
cpg	605.28	J/mol×K	779.92	Joback Method
cpg	617.56	J/mol×K	812.36	Joback Method
cpg	629.07	J/mol×K	844.80	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=U299744&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