l-Leucine, N-(2,3,4-trifluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C14H16F3NO3/c1-7(2)6-10(14(20)21-3)18-13(19)8-4-5-9(15)12(17)11(8)16/h4

InchiKey: BAQHQMFIWKBOKW-UHFFFAOYSA-N

Formula: C14H16F3NO3

SMILES: COC(=O)C(CC(C)C)NC(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 303.28

Physical Properties

Property code	Value	Unit	Source
gf	-712.24	kJ/mol	Joback Method
hf	-1032.97	kJ/mol	Joback Method
hfus	36.57	kJ/mol	Joback Method
hvap	70.13	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	2.421		Crippen Method
mcvol	208.660	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
rinpol	1745.00		NIST Webbook
tb	738.60	K	Joback Method
tc	933.25	K	Joback Method
tf	458.04	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.59	J/mol×K	738.60	Joback Method
cpg	602.30	J/mol×K	771.04	Joback Method
cpg	614.21	J/mol×K	803.48	Joback Method
cpg	625.31	J/mol×K	835.92	Joback Method
cpg	635.63	J/mol×K	868.37	Joback Method
cpg	645.18	J/mol×K	900.81	Joback Method
cpg	653.95	J/mol×K	933.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299630&Units=SI

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