l-Leucine, n-pentafluoropropionyl-, butyl ester

Inchi: InChI=1S/C13H20F5NO3/c1-4-5-6-22-10(20)9(7-8(2)3)19-11(21)12(14,15)13(16,17)18/h
InchiKey: VTKRPSTXBNEJRS-UHFFFAOYSA-N
Formula: C13H20F5NO3
SMILES: CCCCOC(=O)C(CC(C)C)NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 333.29

Physical Properties

Property code	Value	Unit	Source
gf	-1188.12	kJ/mol	Joback Method
hf	-1624.17	kJ/mol	Joback Method
hfus	32.44	kJ/mol	Joback Method
hvap	59.42	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.058		Crippen Method
mcvol	221.870	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	1368.00		NIST Webbook
rinpol	1368.00		NIST Webbook
tb	666.18	K	Joback Method
tc	835.82	K	Joback Method
tf	388.81	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.42	J/mol×K	666.18	Joback Method
cpg	657.17	J/mol×K	694.45	Joback Method
cpg	670.13	J/mol×K	722.73	Joback Method
cpg	682.34	J/mol×K	751.00	Joback Method
cpg	693.84	J/mol×K	779.27	Joback Method
cpg	704.65	J/mol×K	807.55	Joback Method
cpg	714.82	J/mol×K	835.82	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=U321008&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