l-Leucine, n-heptafluorobutyryl-, butyl ester

Inchi: InChI=1S/C14H20F7NO3/c1-4-5-6-25-10(23)9(7-8(2)3)22-11(24)12(15,16)13(17,18)14(1
InchiKey: DQNQXBWJRDSSEK-UHFFFAOYSA-N
Formula: C14H20F7NO3
SMILES: CCCCOC(=O)C(CC(C)C)NC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 383.30

Physical Properties

Property code	Value	Unit	Source
gf	-1566.48	kJ/mol	Joback Method
hf	-2045.78	kJ/mol	Joback Method
hfus	33.77	kJ/mol	Joback Method
hvap	58.71	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.693		Crippen Method
mcvol	239.500	ml/mol	McGowan Method
pc	1390.22	kPa	Joback Method
rinpol	1397.00		NIST Webbook
rinpol	1397.00		NIST Webbook
tb	684.37	K	Joback Method
tc	850.86	K	Joback Method
tf	403.68	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.56	J/mol×K	684.37	Joback Method
cpg	729.16	J/mol×K	712.12	Joback Method
cpg	741.94	J/mol×K	739.87	Joback Method
cpg	753.94	J/mol×K	767.61	Joback Method
cpg	765.22	J/mol×K	795.36	Joback Method
cpg	775.80	J/mol×K	823.11	Joback Method
cpg	785.74	J/mol×K	850.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320992&Units=SI
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

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