l-Leucine, n-heptafluorobutyryl-, isobutyl ester

Inchi: InChI=1S/C14H20F7NO3/c1-7(2)5-9(10(23)25-6-8(3)4)22-11(24)12(15,16)13(17,18)14(1
InchiKey: IXCYRBAXLXHEPV-UHFFFAOYSA-N
Formula: C14H20F7NO3
SMILES: CC(C)COC(=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	-1568.92	kJ/mol	Joback Method
hf	-2051.06	kJ/mol	Joback Method
hfus	30.25	kJ/mol	Joback Method
hvap	58.33	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.549		Crippen Method
mcvol	239.500	ml/mol	McGowan Method
pc	1398.55	kPa	Joback Method
rinpol	1365.00		NIST Webbook
tb	683.93	K	Joback Method
tc	852.09	K	Joback Method
tf	388.68	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.05	J/mol×K	683.93	Joback Method
cpg	729.82	J/mol×K	711.96	Joback Method
cpg	742.74	J/mol×K	739.98	Joback Method
cpg	754.86	J/mol×K	768.01	Joback Method
cpg	766.23	J/mol×K	796.04	Joback Method
cpg	776.90	J/mol×K	824.07	Joback Method
cpg	786.90	J/mol×K	852.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320991&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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