l-Leucine, n-heptafluorobutyryl-, isohexyl ester

Inchi: InChI=1S/C16H24F7NO3/c1-9(2)6-5-7-27-12(25)11(8-10(3)4)24-13(26)14(17,18)15(19,2

InchiKey: LOUVARWAJBNSHR-UHFFFAOYSA-N

Formula: C16H24F7NO3

SMILES: CC(C)CCCOC(=O)C(CC(C)C)NC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 411.36

Physical Properties

Property code	Value	Unit	Source
gf	-1552.08	kJ/mol	Joback Method
hf	-2092.34	kJ/mol	Joback Method
hfus	35.43	kJ/mol	Joback Method
hvap	62.78	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.330		Crippen Method
mcvol	267.680	ml/mol	McGowan Method
pc	1217.44	kPa	Joback Method
rinpol	1528.00		NIST Webbook
tb	729.69	K	Joback Method
tc	900.62	K	Joback Method
tf	411.22	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.23	J/mol×K	729.69	Joback Method
cpg	840.76	J/mol×K	758.18	Joback Method
cpg	854.42	J/mol×K	786.67	Joback Method
cpg	867.24	J/mol×K	815.15	Joback Method
cpg	879.27	J/mol×K	843.64	Joback Method
cpg	890.58	J/mol×K	872.13	Joback Method
cpg	901.21	J/mol×K	900.62	Joback Method

Sources

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=U320994&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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