l-Isoleucine, n-pentafluoropropionyl-, hexyl ester

Inchi: InChI=1S/C15H24F5NO3/c1-4-6-7-8-9-24-12(22)11(10(3)5-2)21-13(23)14(16,17)15(18,1

InchiKey: PHWUWMNSIIRYMW-UHFFFAOYSA-N

Formula: C15H24F5NO3

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

Mol. weight [g/mol]: 361.35

Physical Properties

Property code	Value	Unit	Source
gf	-1171.28	kJ/mol	Joback Method
hf	-1665.45	kJ/mol	Joback Method
hfus	37.62	kJ/mol	Joback Method
hvap	63.87	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.838		Crippen Method
mcvol	250.050	ml/mol	McGowan Method
pc	1364.66	kPa	Joback Method
rinpol	1553.00		NIST Webbook
tb	711.94	K	Joback Method
tc	883.04	K	Joback Method
tf	411.35	K	Joback Method
vc	0.997	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.17	J/mol×K	711.94	Joback Method
cpg	766.75	J/mol×K	740.46	Joback Method
cpg	780.50	J/mol×K	768.97	Joback Method
cpg	793.46	J/mol×K	797.49	Joback Method
cpg	805.66	J/mol×K	826.01	Joback Method
cpg	817.15	J/mol×K	854.52	Joback Method
cpg	827.96	J/mol×K	883.04	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=U320868&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