l-Isoleucine, n-heptafluorobutyryl-, undecyl ester

Inchi: InChI=1S/C21H34F7NO3/c1-4-6-7-8-9-10-11-12-13-14-32-17(30)16(15(3)5-2)29-18(31)1

InchiKey: GXITUHIOQGMVAA-UHFFFAOYSA-N

Formula: C21H34F7NO3

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

Mol. weight [g/mol]: 481.49

Physical Properties

Property code	Value	Unit	Source
gf	-1507.54	kJ/mol	Joback Method
hf	-2190.26	kJ/mol	Joback Method
hfus	51.90	kJ/mol	Joback Method
hvap	74.30	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	6.424		Crippen Method
mcvol	338.130	ml/mol	McGowan Method
pc	888.94	kPa	Joback Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		NIST Webbook
tb	844.53	K	Joback Method
tc	1034.48	K	Joback Method
tf	482.57	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1117.35	J/mol×K	844.53	Joback Method
cpg	1134.28	J/mol×K	876.19	Joback Method
cpg	1150.15	J/mol×K	907.85	Joback Method
cpg	1165.06	J/mol×K	939.50	Joback Method
cpg	1179.08	J/mol×K	971.16	Joback Method
cpg	1192.29	J/mol×K	1002.82	Joback Method
cpg	1204.78	J/mol×K	1034.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320930&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