l-Isoleucine, n-pentafluoropropionyl-, isobutyl ester

Inchi: InChI=1S/C13H20F5NO3/c1-5-8(4)9(10(20)22-6-7(2)3)19-11(21)12(14,15)13(16,17)18/h

InchiKey: ASHLEKATHZTOSX-UHFFFAOYSA-N

Formula: C13H20F5NO3

SMILES: CCC(C)C(NC(=O)C(F)(F)C(F)(F)F)C(=O)OCC(C)C

Mol. weight [g/mol]: 333.29

Physical Properties

Property code	Value	Unit	Source
gf	-1190.56	kJ/mol	Joback Method
hf	-1629.45	kJ/mol	Joback Method
hfus	28.91	kJ/mol	Joback Method
hvap	59.03	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.914		Crippen Method
mcvol	221.870	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	1344.00		NIST Webbook
rinpol	1344.00		NIST Webbook
tb	665.74	K	Joback Method
tc	837.48	K	Joback Method
tf	373.81	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.89	J/mol×K	665.74	Joback Method
cpg	657.84	J/mol×K	694.36	Joback Method
cpg	670.98	J/mol×K	722.99	Joback Method
cpg	683.35	J/mol×K	751.61	Joback Method
cpg	694.97	J/mol×K	780.23	Joback Method
cpg	705.89	J/mol×K	808.86	Joback Method
cpg	716.13	J/mol×K	837.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320866&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