l-Isoleucine, n-pentafluoropropionyl-, propyl ester

Inchi: InChI=1S/C12H18F5NO3/c1-4-6-21-9(19)8(7(3)5-2)18-10(20)11(13,14)12(15,16)17/h7-8
InchiKey: OTRXXZBZQQSDKQ-UHFFFAOYSA-N
Formula: C12H18F5NO3
SMILES: CCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)F)C(C)CC
Mol. weight [g/mol]: 319.27

Physical Properties

Property code	Value	Unit	Source
gf	-1196.54	kJ/mol	Joback Method
hf	-1603.53	kJ/mol	Joback Method
hfus	29.85	kJ/mol	Joback Method
hvap	57.19	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.668		Crippen Method
mcvol	207.780	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	1303.00		NIST Webbook
tb	643.30	K	Joback Method
tc	812.90	K	Joback Method
tf	377.54	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.84	J/mol×K	643.30	Joback Method
cpg	604.14	J/mol×K	671.57	Joback Method
cpg	616.68	J/mol×K	699.83	Joback Method
cpg	628.49	J/mol×K	728.10	Joback Method
cpg	639.60	J/mol×K	756.37	Joback Method
cpg	650.05	J/mol×K	784.63	Joback Method
cpg	659.86	J/mol×K	812.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320865&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