L-Isoleucine, N-trifluoroacetyl-, 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C11H13F8NO3/c1-3-5(2)6(20-8(22)10(14,15)16)7(21)23-4-9(12,13)11(17,18)1

InchiKey: VFODLROYLQBXDL-UHFFFAOYSA-N

Formula: C11H13F8NO3

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

Mol. weight [g/mol]: 359.21

Physical Properties

Property code	Value	Unit	Source
gf	-1786.55	kJ/mol	Joback Method
hf	-2179.97	kJ/mol	Joback Method
hfus	29.08	kJ/mol	Joback Method
hvap	51.22	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.820		Crippen Method
mcvol	199.000	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	1074.70		NIST Webbook
tb	615.00	K	Joback Method
tc	775.00	K	Joback Method
tf	370.46	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.98	J/mol×K	615.00	Joback Method
cpg	578.91	J/mol×K	641.67	Joback Method
cpg	590.11	J/mol×K	668.33	Joback Method
cpg	600.60	J/mol×K	695.00	Joback Method
cpg	610.43	J/mol×K	721.67	Joback Method
cpg	619.64	J/mol×K	748.33	Joback Method
cpg	628.25	J/mol×K	775.00	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=U352352&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