l-Isoleucine, n-heptafluorobutyryl-, nonyl ester

Inchi: InChI=1S/C19H30F7NO3/c1-4-6-7-8-9-10-11-12-30-15(28)14(13(3)5-2)27-16(29)17(20,2
InchiKey: SPLZTJSKVYXGAK-UHFFFAOYSA-N
Formula: C19H30F7NO3
SMILES: CCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)CC
Mol. weight [g/mol]: 453.44

Physical Properties

Property code	Value	Unit	Source
gf	-1524.38	kJ/mol	Joback Method
hf	-2148.98	kJ/mol	Joback Method
hfus	46.72	kJ/mol	Joback Method
hvap	69.84	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	5.644		Crippen Method
mcvol	309.950	ml/mol	McGowan Method
pc	1000.18	kPa	Joback Method
rinpol	1847.00		NIST Webbook
tb	798.77	K	Joback Method
tc	978.27	K	Joback Method
tf	460.03	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.20	J/mol×K	798.77	Joback Method
cpg	1014.00	J/mol×K	828.69	Joback Method
cpg	1028.84	J/mol×K	858.60	Joback Method
cpg	1042.78	J/mol×K	888.52	Joback Method
cpg	1055.90	J/mol×K	918.44	Joback Method
cpg	1068.25	J/mol×K	948.36	Joback Method
cpg	1079.90	J/mol×K	978.27	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=U320928&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