l-Leucine, n-pentafluoropropionyl-, undecyl ester

Inchi: InChI=1S/C20H34F5NO3/c1-4-5-6-7-8-9-10-11-12-13-29-17(27)16(14-15(2)3)26-18(28)1

InchiKey: IBAIABOQWZCHDE-UHFFFAOYSA-N

Formula: C20H34F5NO3

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

Mol. weight [g/mol]: 431.48

Physical Properties

Property code	Value	Unit	Source
gf	-1129.18	kJ/mol	Joback Method
hf	-1768.65	kJ/mol	Joback Method
hfus	50.57	kJ/mol	Joback Method
hvap	75.00	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.789		Crippen Method
mcvol	320.500	ml/mol	McGowan Method
pc	984.55	kPa	Joback Method
rinpol	2008.00		NIST Webbook
rinpol	2008.00		NIST Webbook
tb	826.34	K	Joback Method
tc	1011.76	K	Joback Method
tf	467.70	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.61	J/mol×K	826.34	Joback Method
cpg	1058.45	J/mol×K	857.24	Joback Method
cpg	1074.28	J/mol×K	888.15	Joback Method
cpg	1089.14	J/mol×K	919.05	Joback Method
cpg	1103.10	J/mol×K	949.95	Joback Method
cpg	1116.21	J/mol×K	980.85	Joback Method
cpg	1128.54	J/mol×K	1011.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321013&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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