l-Leucine-, n-pentafluoropropionyl-, decyl ester

Inchi: InChI=1S/C19H32F5NO3/c1-4-5-6-7-8-9-10-11-12-28-16(26)15(13-14(2)3)25-17(27)18(2
InchiKey: VTRVQLGZJQWGJG-UHFFFAOYSA-N
Formula: C19H32F5NO3
SMILES: CCCCCCCCCCOC(=O)C(CC(C)C)NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 417.45

Physical Properties

Property code	Value	Unit	Source
gf	-1137.60	kJ/mol	Joback Method
hf	-1748.01	kJ/mol	Joback Method
hfus	47.98	kJ/mol	Joback Method
hvap	72.77	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.399		Crippen Method
mcvol	306.410	ml/mol	McGowan Method
pc	1046.65	kPa	Joback Method
rinpol	1912.00		NIST Webbook
rinpol	1912.00		NIST Webbook
tb	803.46	K	Joback Method
tc	984.55	K	Joback Method
tf	456.43	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	981.98	J/mol×K	803.46	Joback Method
cpg	998.31	J/mol×K	833.64	Joback Method
cpg	1013.67	J/mol×K	863.82	Joback Method
cpg	1028.12	J/mol×K	894.01	Joback Method
cpg	1041.70	J/mol×K	924.19	Joback Method
cpg	1054.47	J/mol×K	954.37	Joback Method
cpg	1066.48	J/mol×K	984.55	Joback Method

Sources

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=U321012&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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