L-Isoleucine, N-pentafluoropropionyl-, heptadecyl ester

Inchi: InChI=1S/C26H46F5NO3/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-35-23(33)22(
InchiKey: PTDFUKZESFXECJ-UHFFFAOYSA-N
Formula: C26H46F5NO3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)F)C(C)CC
Mol. weight [g/mol]: 515.65

Physical Properties

Property code	Value	Unit	Source
hf	-2052.01	kJ/mol	Cheméo Relay (1.0)
hfus	66.11	kJ/mol	Joback Method
hvap	120.12	kJ/mol	Cheméo Relay (1.0)
log10ws	-8.17		Cheméo Relay (1.0)
logp	8.130		Crippen Method
mcvol	405.040	ml/mol	McGowan Method
rinpol	2595.00		NIST Webbook
rinpol	2595.00		NIST Webbook
tb	624.33	K	Cheméo Relay (1.0)
tf	343.60	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1413.61	J/mol×K	963.62	Joback Method
cpg	1434.72	J/mol×K	1002.34	Joback Method
cpg	1454.32	J/mol×K	1041.05	Joback Method
cpg	1472.57	J/mol×K	1079.77	Joback Method
cpg	1489.60	J/mol×K	1118.48	Joback Method
cpg	1505.56	J/mol×K	1157.20	Joback Method
cpg	1520.59	J/mol×K	1195.91	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320876&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point