L-isoleucine, n-pentafluoropropionyl-, octyl ester

Inchi: InChI=1S/C17H28F5NO3/c1-4-6-7-8-9-10-11-26-14(24)13(12(3)5-2)23-15(25)16(18,19)1

InchiKey: BEJLBMIUOWYOGI-UHFFFAOYSA-N

Formula: C17H28F5NO3

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

Mol. weight [g/mol]: 389.40

Physical Properties

Property code	Value	Unit	Source
hf	-1875.64	kJ/mol	Cheméo Relay (1.0)
hfus	42.80	kJ/mol	Joback Method
hvap	84.16	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.63		Cheméo Relay (1.0)
logp	4.619		Crippen Method
mcvol	278.230	ml/mol	McGowan Method
rinpol	1737.00		NIST Webbook
tb	541.76	K	Cheméo Relay (1.0)
tf	314.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.20	J/mol×K	757.70	Joback Method
cpg	880.62	J/mol×K	786.83	Joback Method
cpg	895.15	J/mol×K	815.95	Joback Method
cpg	908.83	J/mol×K	845.08	Joback Method
cpg	921.71	J/mol×K	874.21	Joback Method
cpg	933.83	J/mol×K	903.33	Joback Method
cpg	945.23	J/mol×K	932.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320870&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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