L-isoleucine, n-pentafluoropropionyl-, ethyl ester

Inchi: InChI=1S/C11H16F5NO3/c1-4-6(3)7(8(18)20-5-2)17-9(19)10(12,13)11(14,15)16/h6-7H,4

InchiKey: LDXFANWPWFYUNP-UHFFFAOYSA-N

Formula: C11H16F5NO3

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

Mol. weight [g/mol]: 305.24

Physical Properties

Property code	Value	Unit	Source
af	0.5804		Cheméo Relay (1.0)
hf	-1759.62	kJ/mol	Cheméo Relay (1.0)
hfus	27.26	kJ/mol	Joback Method
hvap	67.74	kJ/mol	Cheméo Relay (1.0)
logp	2.278		Crippen Method
mcvol	193.690	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	1209.00		NIST Webbook
tb	469.23	K	Cheméo Relay (1.0)
tc	618.51	K	Cheméo Relay (1.0)
tf	305.75	K	Cheméo Relay (1.0)
vc	0.685	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.55	J/mol×K	620.42	Joback Method
cpg	552.38	J/mol×K	648.74	Joback Method
cpg	564.47	J/mol×K	677.07	Joback Method
cpg	575.85	J/mol×K	705.39	Joback Method
cpg	586.55	J/mol×K	733.72	Joback Method
cpg	596.59	J/mol×K	762.04	Joback Method
cpg	606.02	J/mol×K	790.36	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=U320864&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

af:	Acentric Factor
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
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