L-isoleucine, n-pentafluoropropionyl-, pentadecyl ester

Inchi: InChI=1S/C24H42F5NO3/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-33-21(31)20(19(3)5-

InchiKey: KHOLERYBJWHMLD-UHFFFAOYSA-N

Formula: C24H42F5NO3

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

Mol. weight [g/mol]: 487.59

Physical Properties

Property code	Value	Unit	Source
hf	-2013.20	kJ/mol	Cheméo Relay (1.0)
hfus	60.93	kJ/mol	Joback Method
hvap	112.42	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.62		Cheméo Relay (1.0)
logp	7.349		Crippen Method
mcvol	376.860	ml/mol	McGowan Method
rinpol	2409.00		NIST Webbook
tb	608.03	K	Cheméo Relay (1.0)
tf	339.41	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1287.22	J/mol×K	917.86	Joback Method
cpg	1306.62	J/mol×K	953.21	Joback Method
cpg	1324.71	J/mol×K	988.57	Joback Method
cpg	1341.62	J/mol×K	1023.92	Joback Method
cpg	1357.42	J/mol×K	1059.28	Joback Method
cpg	1372.24	J/mol×K	1094.63	Joback Method
cpg	1386.16	J/mol×K	1129.98	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320874&Units=SI

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