l-Isoleucine, n-pentafluoropropionyl-, hexadecyl ester

Inchi: InChI=1S/C25H44F5NO3/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-34-22(32)21(20(3

InchiKey: WAHNKKFSYAEGJO-UHFFFAOYSA-N

Formula: C25H44F5NO3

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

Mol. weight [g/mol]: 501.61

Physical Properties

Property code	Value	Unit	Source
gf	-1087.08	kJ/mol	Joback Method
hf	-1871.85	kJ/mol	Joback Method
hfus	63.52	kJ/mol	Joback Method
hvap	86.13	kJ/mol	Joback Method
log10ws	-8.96		Crippen Method
logp	7.739		Crippen Method
mcvol	390.950	ml/mol	McGowan Method
pc	743.67	kPa	Joback Method
rinpol	2506.00		NIST Webbook
rinpol	2506.00		NIST Webbook
tb	940.74	K	Joback Method
tc	1162.30	K	Joback Method
tf	524.05	K	Joback Method
vc	1.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1350.15	J/mol×K	940.74	Joback Method
cpg	1370.36	J/mol×K	977.67	Joback Method
cpg	1389.17	J/mol×K	1014.59	Joback Method
cpg	1406.71	J/mol×K	1051.52	Joback Method
cpg	1423.10	J/mol×K	1088.45	Joback Method
cpg	1438.45	J/mol×K	1125.38	Joback Method
cpg	1452.89	J/mol×K	1162.30	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=U320875&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