l-Isoleucine, n-pentafluoropropionyl-, octadecyl ester

Inchi: InChI=1S/C27H48F5NO3/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-36-24(34)2

InchiKey: WGPGNDUOQQLCIQ-UHFFFAOYSA-N

Formula: C27H48F5NO3

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

Mol. weight [g/mol]: 529.67

Physical Properties

Property code	Value	Unit	Source
gf	-1070.24	kJ/mol	Joback Method
hf	-1913.13	kJ/mol	Joback Method
hfus	68.70	kJ/mol	Joback Method
hvap	90.58	kJ/mol	Joback Method
log10ws	-9.80		Crippen Method
logp	8.520		Crippen Method
mcvol	419.130	ml/mol	McGowan Method
pc	671.51	kPa	Joback Method
rinpol	2697.00		NIST Webbook
tb	986.50	K	Joback Method
tc	1230.92	K	Joback Method
tf	546.59	K	Joback Method
vc	1.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1477.56	J/mol×K	986.50	Joback Method
cpg	1499.66	J/mol×K	1027.24	Joback Method
cpg	1520.15	J/mol×K	1067.97	Joback Method
cpg	1539.18	J/mol×K	1108.71	Joback Method
cpg	1556.93	J/mol×K	1149.45	Joback Method
cpg	1573.58	J/mol×K	1190.19	Joback Method
cpg	1589.29	J/mol×K	1230.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320877&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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