l-Leucine, n-heptafluorobutyryl-, dodecyl ester

Inchi: InChI=1S/C22H36F7NO3/c1-4-5-6-7-8-9-10-11-12-13-14-33-18(31)17(15-16(2)3)30-19(3
InchiKey: LQGCHSLGQVKGST-UHFFFAOYSA-N
Formula: C22H36F7NO3
SMILES: CCCCCCCCCCCCOC(=O)C(CC(C)C)NC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 495.51

Physical Properties

Property code	Value	Unit	Source
gf	-1499.12	kJ/mol	Joback Method
hf	-2210.90	kJ/mol	Joback Method
hfus	54.49	kJ/mol	Joback Method
hvap	76.52	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	6.814		Crippen Method
mcvol	352.220	ml/mol	McGowan Method
pc	840.16	kPa	Joback Method
rinpol	2115.00		NIST Webbook
tb	867.41	K	Joback Method
tc	1063.99	K	Joback Method
tf	493.84	K	Joback Method
vc	1.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1178.02	J/mol×K	867.41	Joback Method
cpg	1195.60	J/mol×K	900.17	Joback Method
cpg	1212.08	J/mol×K	932.94	Joback Method
cpg	1227.53	J/mol×K	965.70	Joback Method
cpg	1242.07	J/mol×K	998.46	Joback Method
cpg	1255.78	J/mol×K	1031.22	Joback Method
cpg	1268.75	J/mol×K	1063.99	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321001&Units=SI

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