l-Isoleucine, n-heptafluorobutyryl-, hexadecyl ester

Inchi: InChI=1S/C26H44F7NO3/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-37-22(35)21(20(3
InchiKey: VNGXWCCPKWIZGQ-UHFFFAOYSA-N
Formula: C26H44F7NO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)CC
Mol. weight [g/mol]: 551.62

Physical Properties

Property code	Value	Unit	Source
gf	-1465.44	kJ/mol	Joback Method
hf	-2293.46	kJ/mol	Joback Method
hfus	64.85	kJ/mol	Joback Method
hvap	85.42	kJ/mol	Joback Method
log10ws	-9.69		Crippen Method
logp	8.375		Crippen Method
mcvol	408.580	ml/mol	McGowan Method
pc	680.29	kPa	Joback Method
rinpol	2511.00		NIST Webbook
tb	958.93	K	Joback Method
tc	1193.35	K	Joback Method
tf	538.92	K	Joback Method
vc	1.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1427.06	J/mol×K	958.93	Joback Method
cpg	1448.06	J/mol×K	998.00	Joback Method
cpg	1467.66	J/mol×K	1037.07	Joback Method
cpg	1486.02	J/mol×K	1076.14	Joback Method
cpg	1503.33	J/mol×K	1115.21	Joback Method
cpg	1519.75	J/mol×K	1154.28	Joback Method
cpg	1535.47	J/mol×K	1193.35	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=U320933&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