l-Valine, n-heptafluorobutyryl-, isohexyl ester

Inchi: InChI=1S/C15H22F7NO3/c1-8(2)6-5-7-26-11(24)10(9(3)4)23-12(25)13(16,17)14(18,19)1
InchiKey: ZAMRNBRCTJEGMS-UHFFFAOYSA-N
Formula: C15H22F7NO3
SMILES: CC(C)CCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 397.33

Physical Properties

Property code	Value	Unit	Source
gf	-1560.50	kJ/mol	Joback Method
hf	-2071.70	kJ/mol	Joback Method
hfus	32.84	kJ/mol	Joback Method
hvap	60.55	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.939		Crippen Method
mcvol	253.590	ml/mol	McGowan Method
pc	1303.29	kPa	Joback Method
rinpol	1469.00		NIST Webbook
rinpol	1469.00		NIST Webbook
tb	706.81	K	Joback Method
tc	876.08	K	Joback Method
tf	399.95	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.61	J/mol×K	706.81	Joback Method
cpg	784.76	J/mol×K	735.02	Joback Method
cpg	798.05	J/mol×K	763.23	Joback Method
cpg	810.52	J/mol×K	791.45	Joback Method
cpg	822.23	J/mol×K	819.66	Joback Method
cpg	833.21	J/mol×K	847.87	Joback Method
cpg	843.53	J/mol×K	876.08	Joback Method

Sources

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=U320898&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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