l-Valine, n-heptafluorobutyryl-, undecyl ester

Inchi: InChI=1S/C20H32F7NO3/c1-4-5-6-7-8-9-10-11-12-13-31-16(29)15(14(2)3)28-17(30)18(2
InchiKey: DKHTULIZUHGFNE-UHFFFAOYSA-N
Formula: C20H32F7NO3
SMILES: CCCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 467.46

Physical Properties

Property code	Value	Unit	Source
gf	-1515.96	kJ/mol	Joback Method
hf	-2169.62	kJ/mol	Joback Method
hfus	49.31	kJ/mol	Joback Method
hvap	72.07	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.034		Crippen Method
mcvol	324.040	ml/mol	McGowan Method
pc	942.10	kPa	Joback Method
rinpol	1977.00		NIST Webbook
tb	821.65	K	Joback Method
tc	1005.93	K	Joback Method
tf	471.30	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.39	J/mol×K	821.65	Joback Method
cpg	1073.73	J/mol×K	852.36	Joback Method
cpg	1089.06	J/mol×K	883.08	Joback Method
cpg	1103.47	J/mol×K	913.79	Joback Method
cpg	1117.01	J/mol×K	944.51	Joback Method
cpg	1129.78	J/mol×K	975.22	Joback Method
cpg	1141.83	J/mol×K	1005.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320902&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