l-Valine, n-heptafluorobutyryl-, propyl ester

Inchi: InChI=1S/C12H16F7NO3/c1-4-5-23-8(21)7(6(2)3)20-9(22)10(13,14)11(15,16)12(17,18)1
InchiKey: WSTNRUHXTIIYGL-UHFFFAOYSA-N
Formula: C12H16F7NO3
SMILES: CCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 355.25

Physical Properties

Property code	Value	Unit	Source
gf	-1583.32	kJ/mol	Joback Method
hf	-2004.50	kJ/mol	Joback Method
hfus	28.59	kJ/mol	Joback Method
hvap	54.26	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	2.913		Crippen Method
mcvol	211.320	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	1257.00		NIST Webbook
rinpol	1257.00		NIST Webbook
tb	638.61	K	Joback Method
tc	803.83	K	Joback Method
tf	381.14	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.87	J/mol×K	638.61	Joback Method
cpg	622.65	J/mol×K	666.15	Joback Method
cpg	634.65	J/mol×K	693.68	Joback Method
cpg	645.89	J/mol×K	721.22	Joback Method
cpg	656.43	J/mol×K	748.76	Joback Method
cpg	666.30	J/mol×K	776.30	Joback Method
cpg	675.55	J/mol×K	803.83	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=U320894&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