l-Valine, n-pentafluoropropionyl-, isobutyl ester

Inchi: InChI=1S/C12H18F5NO3/c1-6(2)5-21-9(19)8(7(3)4)18-10(20)11(13,14)12(15,16)17/h6-8
InchiKey: WUZWOHTXIXAPDX-UHFFFAOYSA-N
Formula: C12H18F5NO3
SMILES: CC(C)COC(=O)C(NC(=O)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 319.27

Physical Properties

Property code	Value	Unit	Source
gf	-1198.98	kJ/mol	Joback Method
hf	-1608.81	kJ/mol	Joback Method
hfus	26.32	kJ/mol	Joback Method
hvap	56.80	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.524		Crippen Method
mcvol	207.780	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	1274.00		NIST Webbook
rinpol	1274.00		NIST Webbook
tb	642.86	K	Joback Method
tc	814.79	K	Joback Method
tf	362.54	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.29	J/mol×K	642.86	Joback Method
cpg	604.82	J/mol×K	671.52	Joback Method
cpg	617.55	J/mol×K	700.17	Joback Method
cpg	629.53	J/mol×K	728.83	Joback Method
cpg	640.78	J/mol×K	757.48	Joback Method
cpg	651.34	J/mol×K	786.14	Joback Method
cpg	661.25	J/mol×K	814.79	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=U320880&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