l-Valine, n-pentafluoropropionyl-, nonyl ester

Inchi: InChI=1S/C17H28F5NO3/c1-4-5-6-7-8-9-10-11-26-14(24)13(12(2)3)23-15(25)16(18,19)1
InchiKey: OSOLVSYVJHKPIN-UHFFFAOYSA-N
Formula: C17H28F5NO3
SMILES: CCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 389.40

Physical Properties

Property code	Value	Unit	Source
gf	-1154.44	kJ/mol	Joback Method
hf	-1706.73	kJ/mol	Joback Method
hfus	42.80	kJ/mol	Joback Method
hvap	68.32	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.619		Crippen Method
mcvol	278.230	ml/mol	McGowan Method
pc	1189.88	kPa	Joback Method
rinpol	1757.00		NIST Webbook
tb	757.70	K	Joback Method
tc	932.46	K	Joback Method
tf	433.89	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.20	J/mol×K	757.70	Joback Method
cpg	880.62	J/mol×K	786.83	Joback Method
cpg	895.15	J/mol×K	815.95	Joback Method
cpg	908.83	J/mol×K	845.08	Joback Method
cpg	921.71	J/mol×K	874.21	Joback Method
cpg	933.83	J/mol×K	903.33	Joback Method
cpg	945.23	J/mol×K	932.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320884&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