l-Valine, n-pentafluoropropionyl-, decyl ester

Inchi: InChI=1S/C18H30F5NO3/c1-4-5-6-7-8-9-10-11-12-27-15(25)14(13(2)3)24-16(26)17(19,2
InchiKey: CUQFTSBVZQBCFH-UHFFFAOYSA-N
Formula: C18H30F5NO3
SMILES: CCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 403.43

Physical Properties

Property code	Value	Unit	Source
gf	-1146.02	kJ/mol	Joback Method
hf	-1727.37	kJ/mol	Joback Method
hfus	45.39	kJ/mol	Joback Method
hvap	70.55	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.009		Crippen Method
mcvol	292.320	ml/mol	McGowan Method
pc	1114.82	kPa	Joback Method
rinpol	1849.00		NIST Webbook
tb	780.58	K	Joback Method
tc	958.14	K	Joback Method
tf	445.16	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	923.15	J/mol×K	780.58	Joback Method
cpg	939.02	J/mol×K	810.17	Joback Method
cpg	953.95	J/mol×K	839.77	Joback Method
cpg	968.01	J/mol×K	869.36	Joback Method
cpg	981.23	J/mol×K	898.95	Joback Method
cpg	993.67	J/mol×K	928.55	Joback Method
cpg	1005.37	J/mol×K	958.14	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U320885&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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