l-Valine, n-pentafluoropropionyl-, hexadecyl ester

Inchi: InChI=1S/C24H42F5NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-33-21(31)20(19(2)
InchiKey: RNAIREZAVGOKNI-UHFFFAOYSA-N
Formula: C24H42F5NO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 487.59

Physical Properties

Property code	Value	Unit	Source
gf	-1095.50	kJ/mol	Joback Method
hf	-1851.21	kJ/mol	Joback Method
hfus	60.93	kJ/mol	Joback Method
hvap	83.90	kJ/mol	Joback Method
log10ws	-8.54		Crippen Method
logp	7.349		Crippen Method
mcvol	376.860	ml/mol	McGowan Method
pc	784.19	kPa	Joback Method
rinpol	2429.00		NIST Webbook
tb	917.86	K	Joback Method
tc	1129.98	K	Joback Method
tf	512.78	K	Joback Method
vc	1.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1287.22	J/mol×K	917.86	Joback Method
cpg	1306.62	J/mol×K	953.21	Joback Method
cpg	1324.71	J/mol×K	988.57	Joback Method
cpg	1341.62	J/mol×K	1023.92	Joback Method
cpg	1357.42	J/mol×K	1059.28	Joback Method
cpg	1372.24	J/mol×K	1094.63	Joback Method
cpg	1386.16	J/mol×K	1129.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320890&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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