l-Valine, n-pentafluoropropionyl-, pentadecyl ester

Inchi: InChI=1S/C23H40F5NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-32-20(30)19(18(2)3)2

InchiKey: HTYUIPVJJQHEQW-UHFFFAOYSA-N

Formula: C23H40F5NO3

SMILES: CCCCCCCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)F)C(C)C

Mol. weight [g/mol]: 473.56

Physical Properties

Property code	Value	Unit	Source
gf	-1103.92	kJ/mol	Joback Method
hf	-1830.57	kJ/mol	Joback Method
hfus	58.34	kJ/mol	Joback Method
hvap	81.68	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	6.959		Crippen Method
mcvol	362.770	ml/mol	McGowan Method
pc	828.11	kPa	Joback Method
rinpol	2333.00		NIST Webbook
tb	894.98	K	Joback Method
tc	1098.86	K	Joback Method
tf	501.51	K	Joback Method
vc	1.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1224.86	J/mol×K	894.98	Joback Method
cpg	1243.52	J/mol×K	928.96	Joback Method
cpg	1260.97	J/mol×K	962.94	Joback Method
cpg	1277.29	J/mol×K	996.92	Joback Method
cpg	1292.57	J/mol×K	1030.90	Joback Method
cpg	1306.90	J/mol×K	1064.88	Joback Method
cpg	1320.36	J/mol×K	1098.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320889&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