l-Valine, n-pentafluoropropionyl-, tetradecyl ester

Inchi: InChI=1S/C22H38F5NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-31-19(29)18(17(2)3)28-2
InchiKey: YHZIQORKOBTBCB-UHFFFAOYSA-N
Formula: C22H38F5NO3
SMILES: CCCCCCCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 459.53

Physical Properties

Property code	Value	Unit	Source
gf	-1112.34	kJ/mol	Joback Method
hf	-1809.93	kJ/mol	Joback Method
hfus	55.75	kJ/mol	Joback Method
hvap	79.45	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	6.569		Crippen Method
mcvol	348.680	ml/mol	McGowan Method
pc	875.84	kPa	Joback Method
rinpol	2228.00		NIST Webbook
rinpol	2228.00		NIST Webbook
tb	872.10	K	Joback Method
tc	1068.83	K	Joback Method
tf	490.24	K	Joback Method
vc	1.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1163.10	J/mol×K	872.10	Joback Method
cpg	1181.10	J/mol×K	904.89	Joback Method
cpg	1197.96	J/mol×K	937.68	Joback Method
cpg	1213.75	J/mol×K	970.47	Joback Method
cpg	1228.55	J/mol×K	1003.26	Joback Method
cpg	1242.44	J/mol×K	1036.04	Joback Method
cpg	1255.49	J/mol×K	1068.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320888&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