L-Valine, N-pentafluorobenzoyl-, pentadecyl ester

Inchi: InChI=1S/C27H40F5NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-36-27(35)25(18(2)3)3
InchiKey: PHWQGNNNOMPKAU-UHFFFAOYSA-N
Formula: C27H40F5NO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1c(F)c(F)c(F)c(F)c1F)C(C)C
Mol. weight [g/mol]: 521.60

Physical Properties

Property code	Value	Unit	Source
gf	-1011.66	kJ/mol	Joback Method
hf	-1716.45	kJ/mol	Joback Method
hfus	75.62	kJ/mol	Joback Method
hvap	98.76	kJ/mol	Joback Method
log10ws	-10.16		Crippen Method
logp	7.771		Crippen Method
mcvol	395.370	ml/mol	McGowan Method
pc	754.33	kPa	Joback Method
rinpol	2978.00		NIST Webbook
rinpol	2978.00		NIST Webbook
tb	1044.54	K	Joback Method
tc	1302.07	K	Joback Method
tf	630.77	K	Joback Method
vc	1.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1368.98	J/mol×K	1044.54	Joback Method
cpg	1386.62	J/mol×K	1087.46	Joback Method
cpg	1402.22	J/mol×K	1130.38	Joback Method
cpg	1415.85	J/mol×K	1173.31	Joback Method
cpg	1427.59	J/mol×K	1216.23	Joback Method
cpg	1437.54	J/mol×K	1259.15	Joback Method
cpg	1445.76	J/mol×K	1302.07	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346614&Units=SI

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