L-Valine, N-pentafluorobenzoyl-, hexadecyl ester

Inchi: InChI=1S/C28H42F5NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-37-28(36)26(19(2)
InchiKey: YXVMDVKUMVXQQJ-UHFFFAOYSA-N
Formula: C28H42F5NO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1c(F)c(F)c(F)c(F)c1F)C(C)C
Mol. weight [g/mol]: 535.63

Physical Properties

Property code	Value	Unit	Source
gf	-1003.24	kJ/mol	Joback Method
hf	-1737.09	kJ/mol	Joback Method
hfus	78.21	kJ/mol	Joback Method
hvap	100.98	kJ/mol	Joback Method
log10ws	-10.58		Crippen Method
logp	8.161		Crippen Method
mcvol	409.460	ml/mol	McGowan Method
pc	716.07	kPa	Joback Method
rinpol	3078.00		NIST Webbook
rinpol	3078.00		NIST Webbook
tb	1067.42	K	Joback Method
tc	1338.81	K	Joback Method
tf	642.04	K	Joback Method
vc	1.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1431.63	J/mol×K	1067.42	Joback Method
cpg	1449.86	J/mol×K	1112.65	Joback Method
cpg	1465.80	J/mol×K	1157.88	Joback Method
cpg	1479.56	J/mol×K	1203.11	Joback Method
cpg	1491.26	J/mol×K	1248.35	Joback Method
cpg	1500.98	J/mol×K	1293.58	Joback Method
cpg	1508.83	J/mol×K	1338.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346615&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