L-Valine, N-pentafluorobenzoyl-, dodecyl ester

Inchi: InChI=1S/C24H34F5NO3/c1-4-5-6-7-8-9-10-11-12-13-14-33-24(32)22(15(2)3)30-23(31)1
InchiKey: JCOMMQKSHHBFJZ-UHFFFAOYSA-N
Formula: C24H34F5NO3
SMILES: CCCCCCCCCCCCOC(=O)C(NC(=O)c1c(F)c(F)c(F)c(F)c1F)C(C)C
Mol. weight [g/mol]: 479.52

Physical Properties

Property code	Value	Unit	Source
gf	-1036.92	kJ/mol	Joback Method
hf	-1654.53	kJ/mol	Joback Method
hfus	67.85	kJ/mol	Joback Method
hvap	92.08	kJ/mol	Joback Method
log10ws	-8.90		Crippen Method
logp	6.601		Crippen Method
mcvol	353.100	ml/mol	McGowan Method
pc	889.47	kPa	Joback Method
rinpol	2691.00		NIST Webbook
rinpol	2691.00		NIST Webbook
tb	975.90	K	Joback Method
tc	1200.82	K	Joback Method
tf	596.96	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1183.14	J/mol×K	975.90	Joback Method
cpg	1199.20	J/mol×K	1013.39	Joback Method
cpg	1213.74	J/mol×K	1050.87	Joback Method
cpg	1226.81	J/mol×K	1088.36	Joback Method
cpg	1238.44	J/mol×K	1125.84	Joback Method
cpg	1248.69	J/mol×K	1163.33	Joback Method
cpg	1257.59	J/mol×K	1200.82	Joback Method

Sources

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=U346612&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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