L-Valine, N-pentafluorobenzoyl-, heptyl ester

Inchi: InChI=1S/C19H24F5NO3/c1-4-5-6-7-8-9-28-19(27)17(10(2)3)25-18(26)11-12(20)14(22)1
InchiKey: JDVCMUPEXLLOPF-UHFFFAOYSA-N
Formula: C19H24F5NO3
SMILES: CCCCCCCOC(=O)C(NC(=O)c1c(F)c(F)c(F)c(F)c1F)C(C)C
Mol. weight [g/mol]: 409.39

Physical Properties

Property code	Value	Unit	Source
gf	-1079.02	kJ/mol	Joback Method
hf	-1551.33	kJ/mol	Joback Method
hfus	54.90	kJ/mol	Joback Method
hvap	80.95	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	4.650		Crippen Method
mcvol	282.650	ml/mol	McGowan Method
pc	1211.51	kPa	Joback Method
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
tb	861.50	K	Joback Method
tc	1055.91	K	Joback Method
tf	540.61	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.43	J/mol×K	861.50	Joback Method
cpg	897.28	J/mol×K	893.90	Joback Method
cpg	910.13	J/mol×K	926.30	Joback Method
cpg	921.98	J/mol×K	958.71	Joback Method
cpg	932.87	J/mol×K	991.11	Joback Method
cpg	942.80	J/mol×K	1023.51	Joback Method
cpg	951.79	J/mol×K	1055.91	Joback Method

Sources

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=U346608&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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