L-Valine, N-(2,5-ditrifluoromethylbenzoyl)-, pentyl ester

Inchi: InChI=1S/C19H23F6NO3/c1-4-5-6-9-29-17(28)15(11(2)3)26-16(27)13-10-12(18(20,21)22

InchiKey: WXSJSZLVQDOZMR-UHFFFAOYSA-N

Formula: C19H23F6NO3

SMILES: CCCCCOC(=O)C(NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F)C(C)C

Mol. weight [g/mol]: 427.38

Physical Properties

Property code	Value	Unit	Source
gf	-1239.26	kJ/mol	Joback Method
hf	-1730.53	kJ/mol	Joback Method
hfus	44.32	kJ/mol	Joback Method
hvap	75.56	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	5.212		Crippen Method
mcvol	284.420	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rinpol	1973.00		NIST Webbook
rinpol	1973.00		NIST Webbook
tb	839.37	K	Joback Method
tc	1032.48	K	Joback Method
tf	508.48	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.75	J/mol×K	839.37	Joback Method
cpg	909.36	J/mol×K	871.56	Joback Method
cpg	922.02	J/mol×K	903.74	Joback Method
cpg	933.79	J/mol×K	935.93	Joback Method
cpg	944.73	J/mol×K	968.11	Joback Method
cpg	954.90	J/mol×K	1000.30	Joback Method
cpg	964.37	J/mol×K	1032.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346570&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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