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

Inchi: InChI=1S/C17H19F6NO3/c1-4-7-27-15(26)13(9(2)3)24-14(25)11-8-10(16(18,19)20)5-6-1

InchiKey: DDZILZZWXNQQFP-UHFFFAOYSA-N

Formula: C17H19F6NO3

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

Mol. weight [g/mol]: 399.33

Physical Properties

Property code	Value	Unit	Source
gf	-1256.10	kJ/mol	Joback Method
hf	-1689.25	kJ/mol	Joback Method
hfus	39.14	kJ/mol	Joback Method
hvap	71.10	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	4.432		Crippen Method
mcvol	256.240	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
tb	793.61	K	Joback Method
tc	983.60	K	Joback Method
tf	485.94	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.30	J/mol×K	793.61	Joback Method
cpg	795.21	J/mol×K	825.27	Joback Method
cpg	807.22	J/mol×K	856.94	Joback Method
cpg	818.37	J/mol×K	888.60	Joback Method
cpg	828.73	J/mol×K	920.27	Joback Method
cpg	838.34	J/mol×K	951.93	Joback Method
cpg	847.26	J/mol×K	983.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346568&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