L-Valine, N-(3-trifluoromethylbenzoyl)-, ethyl ester

Inchi: InChI=1S/C15H18F3NO3/c1-4-22-14(21)12(9(2)3)19-13(20)10-6-5-7-11(8-10)15(16,17)1

InchiKey: IXDLVGRQBAUEOT-UHFFFAOYSA-N

Formula: C15H18F3NO3

SMILES: CCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1)C(C)C

Mol. weight [g/mol]: 317.30

Physical Properties

Property code	Value	Unit	Source
gf	-681.72	kJ/mol	Joback Method
hf	-1039.42	kJ/mol	Joback Method
hfus	32.52	kJ/mol	Joback Method
hvap	69.74	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.023		Crippen Method
mcvol	222.750	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	1816.00		NIST Webbook
rinpol	1816.00		NIST Webbook
tb	748.29	K	Joback Method
tc	947.63	K	Joback Method
tf	446.69	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.00	J/mol×K	748.29	Joback Method
cpg	661.54	J/mol×K	781.51	Joback Method
cpg	674.12	J/mol×K	814.74	Joback Method
cpg	685.79	J/mol×K	847.96	Joback Method
cpg	696.60	J/mol×K	881.18	Joback Method
cpg	706.58	J/mol×K	914.40	Joback Method
cpg	715.79	J/mol×K	947.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346715&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