L-Valine, N-(2-trifluoromethylbenzoyl)-, propyl ester

Inchi: InChI=1S/C16H20F3NO3/c1-4-9-23-15(22)13(10(2)3)20-14(21)11-7-5-6-8-12(11)16(17,1

InchiKey: KVSIMTDWFHOFDO-UHFFFAOYSA-N

Formula: C16H20F3NO3

SMILES: CCCOC(=O)C(NC(=O)c1ccccc1C(F)(F)F)C(C)C

Mol. weight [g/mol]: 331.33

Physical Properties

Property code	Value	Unit	Source
gf	-673.30	kJ/mol	Joback Method
hf	-1060.06	kJ/mol	Joback Method
hfus	35.11	kJ/mol	Joback Method
hvap	71.96	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.413		Crippen Method
mcvol	236.840	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	1957.00		NIST Webbook
rinpol	1957.00		NIST Webbook
tb	771.17	K	Joback Method
tc	969.39	K	Joback Method
tf	457.96	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.89	J/mol×K	771.17	Joback Method
cpg	716.73	J/mol×K	804.21	Joback Method
cpg	729.61	J/mol×K	837.24	Joback Method
cpg	741.56	J/mol×K	870.28	Joback Method
cpg	752.63	J/mol×K	903.32	Joback Method
cpg	762.87	J/mol×K	936.35	Joback Method
cpg	772.32	J/mol×K	969.39	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=U346703&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