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

Inchi: InChI=1S/C22H32F3NO3/c1-4-5-6-7-8-9-10-14-29-21(28)19(16(2)3)26-20(27)17-12-11-1

InchiKey: RNWMXMVFTXUHIU-UHFFFAOYSA-N

Formula: C22H32F3NO3

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

Mol. weight [g/mol]: 415.49

Physical Properties

Property code	Value	Unit	Source
gf	-622.78	kJ/mol	Joback Method
hf	-1183.90	kJ/mol	Joback Method
hfus	50.65	kJ/mol	Joback Method
hvap	85.32	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	5.754		Crippen Method
mcvol	321.380	ml/mol	McGowan Method
pc	1117.06	kPa	Joback Method
rinpol	2462.00		NIST Webbook
rinpol	2462.00		NIST Webbook
tb	908.45	K	Joback Method
tc	1113.64	K	Joback Method
tf	525.58	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1050.80	J/mol×K	908.45	Joback Method
cpg	1066.36	J/mol×K	942.65	Joback Method
cpg	1080.79	J/mol×K	976.85	Joback Method
cpg	1094.15	J/mol×K	1011.04	Joback Method
cpg	1106.52	J/mol×K	1045.24	Joback Method
cpg	1117.96	J/mol×K	1079.44	Joback Method
cpg	1128.54	J/mol×K	1113.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346721&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