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

Inchi: InChI=1S/C18H24F3NO3/c1-4-5-6-10-25-17(24)15(12(2)3)22-16(23)13-8-7-9-14(11-13)1

InchiKey: RMRXYJAWYQVLDT-UHFFFAOYSA-N

Formula: C18H24F3NO3

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

Mol. weight [g/mol]: 359.38

Physical Properties

Property code	Value	Unit	Source
gf	-656.46	kJ/mol	Joback Method
hf	-1101.34	kJ/mol	Joback Method
hfus	40.29	kJ/mol	Joback Method
hvap	76.42	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.193		Crippen Method
mcvol	265.020	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	2085.00		NIST Webbook
rinpol	2085.00		NIST Webbook
tb	816.93	K	Joback Method
tc	1014.67	K	Joback Method
tf	480.50	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.56	J/mol×K	816.93	Joback Method
cpg	829.97	J/mol×K	849.89	Joback Method
cpg	843.37	J/mol×K	882.84	Joback Method
cpg	855.81	J/mol×K	915.80	Joback Method
cpg	867.34	J/mol×K	948.76	Joback Method
cpg	878.01	J/mol×K	981.71	Joback Method
cpg	887.88	J/mol×K	1014.67	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=U346717&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