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

Inchi: InChI=1S/C19H26F3NO3/c1-12(2)7-6-10-26-18(25)16(13(3)4)23-17(24)14-8-5-9-15(11-1

InchiKey: HBIPFQSZCNWBIP-UHFFFAOYSA-N

Formula: C19H26F3NO3

SMILES: CC(C)CCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1)C(C)C

Mol. weight [g/mol]: 373.41

Physical Properties

Property code	Value	Unit	Source
gf	-650.48	kJ/mol	Joback Method
hf	-1127.26	kJ/mol	Joback Method
hfus	39.36	kJ/mol	Joback Method
hvap	78.25	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.439		Crippen Method
mcvol	279.110	ml/mol	McGowan Method
pc	1375.82	kPa	Joback Method
rinpol	2123.00		NIST Webbook
rinpol	2123.00		NIST Webbook
tb	839.37	K	Joback Method
tc	1039.48	K	Joback Method
tf	476.77	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.76	J/mol×K	839.37	Joback Method
cpg	888.55	J/mol×K	872.72	Joback Method
cpg	902.28	J/mol×K	906.07	Joback Method
cpg	915.00	J/mol×K	939.42	Joback Method
cpg	926.77	J/mol×K	972.77	Joback Method
cpg	937.65	J/mol×K	1006.12	Joback Method
cpg	947.68	J/mol×K	1039.48	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346718&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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