L-Valine, N-(3-methoxy-2,4,5-trifluorobenzoyl)-, isohexyl ester

Inchi: InChI=1S/C19H26F3NO4/c1-10(2)7-6-8-27-19(25)16(11(3)4)23-18(24)12-9-13(20)15(22)
InchiKey: UUMBDYADFQOBQI-UHFFFAOYSA-N
Formula: C19H26F3NO4
SMILES: COc1c(F)c(F)cc(C(=O)NC(C(=O)OCCCC(C)C)C(C)C)c1F
Mol. weight [g/mol]: 389.41

Physical Properties

Property code	Value	Unit	Source
gf	-787.21	kJ/mol	Joback Method
hf	-1285.14	kJ/mol	Joback Method
hfus	46.79	kJ/mol	Joback Method
hvap	83.95	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	3.846		Crippen Method
mcvol	284.980	ml/mol	McGowan Method
pc	1296.73	kPa	Joback Method
rinpol	2302.00		NIST Webbook
rinpol	2302.00		NIST Webbook
tb	879.96	K	Joback Method
tc	1081.18	K	Joback Method
tf	534.14	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.60	J/mol×K	879.96	Joback Method
cpg	912.67	J/mol×K	913.50	Joback Method
cpg	925.57	J/mol×K	947.03	Joback Method
cpg	937.33	J/mol×K	980.57	Joback Method
cpg	947.95	J/mol×K	1014.11	Joback Method
cpg	957.44	J/mol×K	1047.64	Joback Method
cpg	965.81	J/mol×K	1081.18	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=U346433&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