l-Valine, N-(2,3,4-trifluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C13H14F3NO3/c1-6(2)11(13(19)20-3)17-12(18)7-4-5-8(14)10(16)9(7)15/h4-6,1

InchiKey: QFJZSYCNJXSYHU-UHFFFAOYSA-N

Formula: C13H14F3NO3

SMILES: COC(=O)C(NC(=O)c1ccc(F)c(F)c1F)C(C)C

Mol. weight [g/mol]: 289.25

Physical Properties

Property code	Value	Unit	Source
gf	-720.66	kJ/mol	Joback Method
hf	-1012.33	kJ/mol	Joback Method
hfus	33.98	kJ/mol	Joback Method
hvap	67.91	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	2.031		Crippen Method
mcvol	194.570	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1672.00		NIST Webbook
rinpol	1672.00		NIST Webbook
tb	715.72	K	Joback Method
tc	911.69	K	Joback Method
tf	446.77	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.54	J/mol×K	715.72	Joback Method
cpg	548.80	J/mol×K	748.38	Joback Method
cpg	560.29	J/mol×K	781.04	Joback Method
cpg	571.01	J/mol×K	813.70	Joback Method
cpg	580.98	J/mol×K	846.36	Joback Method
cpg	590.21	J/mol×K	879.02	Joback Method
cpg	598.70	J/mol×K	911.69	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=U299629&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