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

Inchi: InChI=1S/C23H34F3NO4/c1-5-6-7-8-9-10-11-12-13-31-23(29)20(15(2)3)27-22(28)16-14-
InchiKey: AJXLGVOQLSGZHI-UHFFFAOYSA-N
Formula: C23H34F3NO4
SMILES: CCCCCCCCCCOC(=O)C(NC(=O)c1cc(F)c(F)c(OC)c1F)C(C)C
Mol. weight [g/mol]: 445.52

Physical Properties

Property code	Value	Unit	Source
gf	-751.09	kJ/mol	Joback Method
hf	-1362.42	kJ/mol	Joback Method
hfus	60.68	kJ/mol	Joback Method
hvap	93.24	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	5.551		Crippen Method
mcvol	341.340	ml/mol	McGowan Method
pc	995.76	kPa	Joback Method
rinpol	2742.00		NIST Webbook
rinpol	2742.00		NIST Webbook
tb	971.92	K	Joback Method
tc	1191.12	K	Joback Method
tf	594.22	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1137.66	J/mol×K	971.92	Joback Method
cpg	1152.82	J/mol×K	1008.45	Joback Method
cpg	1166.45	J/mol×K	1044.99	Joback Method
cpg	1178.58	J/mol×K	1081.52	Joback Method
cpg	1189.23	J/mol×K	1118.05	Joback Method
cpg	1198.43	J/mol×K	1154.59	Joback Method
cpg	1206.21	J/mol×K	1191.12	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346435&Units=SI

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