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

Inchi: InChI=1S/C24H36F3NO4/c1-5-6-7-8-9-10-11-12-13-14-32-24(30)21(16(2)3)28-23(29)17-
InchiKey: NLKDEOSGFSJNBT-UHFFFAOYSA-N
Formula: C24H36F3NO4
SMILES: CCCCCCCCCCCOC(=O)C(NC(=O)c1cc(F)c(F)c(OC)c1F)C(C)C
Mol. weight [g/mol]: 459.54

Physical Properties

Property code	Value	Unit	Source
gf	-742.67	kJ/mol	Joback Method
hf	-1383.06	kJ/mol	Joback Method
hfus	63.27	kJ/mol	Joback Method
hvap	95.46	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	5.941		Crippen Method
mcvol	355.430	ml/mol	McGowan Method
pc	938.07	kPa	Joback Method
rinpol	2839.00		NIST Webbook
rinpol	2839.00		NIST Webbook
tb	994.80	K	Joback Method
tc	1221.33	K	Joback Method
tf	605.49	K	Joback Method
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1198.81	J/mol×K	994.80	Joback Method
cpg	1214.27	J/mol×K	1032.56	Joback Method
cpg	1228.06	J/mol×K	1070.31	Joback Method
cpg	1240.22	J/mol×K	1108.07	Joback Method
cpg	1250.78	J/mol×K	1145.82	Joback Method
cpg	1259.78	J/mol×K	1183.58	Joback Method
cpg	1267.24	J/mol×K	1221.33	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=U346436&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