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

Inchi: InChI=1S/C20H28F3NO4/c1-5-6-7-8-9-10-28-20(26)17(12(2)3)24-19(25)13-11-14(21)16(
InchiKey: IUQQNBMCZAMLQD-UHFFFAOYSA-N
Formula: C20H28F3NO4
SMILES: CCCCCCCOC(=O)C(NC(=O)c1cc(F)c(F)c(OC)c1F)C(C)C
Mol. weight [g/mol]: 403.44

Physical Properties

Property code	Value	Unit	Source
gf	-776.35	kJ/mol	Joback Method
hf	-1300.50	kJ/mol	Joback Method
hfus	52.91	kJ/mol	Joback Method
hvap	86.56	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	4.380		Crippen Method
mcvol	299.070	ml/mol	McGowan Method
pc	1204.80	kPa	Joback Method
rinpol	2451.00		NIST Webbook
rinpol	2451.00		NIST Webbook
tb	903.28	K	Joback Method
tc	1106.92	K	Joback Method
tf	560.41	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.11	J/mol×K	903.28	Joback Method
cpg	971.41	J/mol×K	937.22	Joback Method
cpg	984.50	J/mol×K	971.16	Joback Method
cpg	996.38	J/mol×K	1005.10	Joback Method
cpg	1007.08	J/mol×K	1039.04	Joback Method
cpg	1016.59	J/mol×K	1072.98	Joback Method
cpg	1024.94	J/mol×K	1106.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346434&Units=SI
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

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