L-Valine, N-(2-fluoro-3-trifluoromethylbenzoyl)-, nonyl ester

Inchi: InChI=1S/C22H31F4NO3/c1-4-5-6-7-8-9-10-14-30-21(29)19(15(2)3)27-20(28)16-12-11-1

InchiKey: GPIVSSUUPKVESG-UHFFFAOYSA-N

Formula: C22H31F4NO3

SMILES: CCCCCCCCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1F)C(C)C

Mol. weight [g/mol]: 433.48

Physical Properties

Property code	Value	Unit	Source
gf	-827.22	kJ/mol	Joback Method
hf	-1391.48	kJ/mol	Joback Method
hfus	53.34	kJ/mol	Joback Method
hvap	85.16	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	5.893		Crippen Method
mcvol	323.150	ml/mol	McGowan Method
pc	1073.57	kPa	Joback Method
rinpol	2447.00		NIST Webbook
rinpol	2447.00		NIST Webbook
tb	912.70	K	Joback Method
tc	1117.72	K	Joback Method
tf	538.69	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.16	J/mol×K	912.70	Joback Method
cpg	1072.44	J/mol×K	946.87	Joback Method
cpg	1086.59	J/mol×K	981.04	Joback Method
cpg	1099.67	J/mol×K	1015.21	Joback Method
cpg	1111.75	J/mol×K	1049.38	Joback Method
cpg	1122.89	J/mol×K	1083.55	Joback Method
cpg	1133.14	J/mol×K	1117.72	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=U346470&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