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

Inchi: InChI=1S/C16H19F4NO3/c1-4-8-24-15(23)13(9(2)3)21-14(22)10-6-5-7-11(12(10)17)16(1

InchiKey: HYWUKRXOYFCEMZ-UHFFFAOYSA-N

Formula: C16H19F4NO3

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

Mol. weight [g/mol]: 349.32

Physical Properties

Property code	Value	Unit	Source
gf	-877.74	kJ/mol	Joback Method
hf	-1267.64	kJ/mol	Joback Method
hfus	37.80	kJ/mol	Joback Method
hvap	71.81	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.552		Crippen Method
mcvol	238.610	ml/mol	McGowan Method
pc	1631.17	kPa	Joback Method
rinpol	1882.00		NIST Webbook
rinpol	1882.00		NIST Webbook
tb	775.42	K	Joback Method
tc	968.98	K	Joback Method
tf	471.07	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.57	J/mol×K	775.42	Joback Method
cpg	722.86	J/mol×K	807.68	Joback Method
cpg	735.23	J/mol×K	839.94	Joback Method
cpg	746.73	J/mol×K	872.20	Joback Method
cpg	757.39	J/mol×K	904.46	Joback Method
cpg	767.26	J/mol×K	936.72	Joback Method
cpg	776.36	J/mol×K	968.98	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=U346464&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