L-Valine, N-(3-fluoro-4-trifluoromethylbenzoyl)-, pentyl ester

Inchi: InChI=1S/C18H23F4NO3/c1-4-5-6-9-26-17(25)15(11(2)3)23-16(24)12-7-8-13(14(19)10-1

InchiKey: AFEQLJGRANJKKP-UHFFFAOYSA-N

Formula: C18H23F4NO3

SMILES: CCCCCOC(=O)C(NC(=O)c1ccc(C(F)(F)F)c(F)c1)C(C)C

Mol. weight [g/mol]: 377.37

Physical Properties

Property code	Value	Unit	Source
gf	-860.90	kJ/mol	Joback Method
hf	-1308.92	kJ/mol	Joback Method
hfus	42.98	kJ/mol	Joback Method
hvap	76.26	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.332		Crippen Method
mcvol	266.790	ml/mol	McGowan Method
pc	1404.84	kPa	Joback Method
rinpol	1996.00		NIST Webbook
rinpol	1996.00		NIST Webbook
tb	821.18	K	Joback Method
tc	1015.63	K	Joback Method
tf	493.61	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.16	J/mol×K	821.18	Joback Method
cpg	836.09	J/mol×K	853.59	Joback Method
cpg	849.06	J/mol×K	886.00	Joback Method
cpg	861.10	J/mol×K	918.40	Joback Method
cpg	872.26	J/mol×K	950.81	Joback Method
cpg	882.58	J/mol×K	983.22	Joback Method
cpg	892.11	J/mol×K	1015.63	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=U346553&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