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

Inchi: InChI=1S/C19H25F4NO3/c1-4-5-6-7-10-27-18(26)16(12(2)3)24-17(25)13-8-9-14(15(20)1

InchiKey: KANKPGFEISFSAZ-UHFFFAOYSA-N

Formula: C19H25F4NO3

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

Mol. weight [g/mol]: 391.40

Physical Properties

Property code	Value	Unit	Source
gf	-852.48	kJ/mol	Joback Method
hf	-1329.56	kJ/mol	Joback Method
hfus	45.57	kJ/mol	Joback Method
hvap	78.49	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	4.722		Crippen Method
mcvol	280.880	ml/mol	McGowan Method
pc	1308.95	kPa	Joback Method
rinpol	2089.00		NIST Webbook
rinpol	2089.00		NIST Webbook
tb	844.06	K	Joback Method
tc	1039.97	K	Joback Method
tf	504.88	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.77	J/mol×K	844.06	Joback Method
cpg	894.02	J/mol×K	876.71	Joback Method
cpg	907.27	J/mol×K	909.36	Joback Method
cpg	919.57	J/mol×K	942.01	Joback Method
cpg	930.96	J/mol×K	974.66	Joback Method
cpg	941.49	J/mol×K	1007.32	Joback Method
cpg	951.21	J/mol×K	1039.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346555&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

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