L-Valine, N-(4-fluorobenzoyl)-, hexyl ester

Inchi: InChI=1S/C18H26FNO3/c1-4-5-6-7-12-23-18(22)16(13(2)3)20-17(21)14-8-10-15(19)11-9

InchiKey: FTDAJLFJNNUSNO-UHFFFAOYSA-N

Formula: C18H26FNO3

SMILES: CCCCCCOC(=O)C(NC(=O)c1ccc(F)cc1)C(C)C

Mol. weight [g/mol]: 323.40

Physical Properties

Property code	Value	Unit	Source
gf	-269.68	kJ/mol	Joback Method
hf	-700.37	kJ/mol	Joback Method
hfus	41.55	kJ/mol	Joback Method
hvap	79.34	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	3.704		Crippen Method
mcvol	261.480	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
rinpol	2238.00		NIST Webbook
rinpol	2238.00		NIST Webbook
tb	821.62	K	Joback Method
tc	1023.37	K	Joback Method
tf	476.90	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.24	J/mol×K	821.62	Joback Method
cpg	814.40	J/mol×K	855.24	Joback Method
cpg	828.50	J/mol×K	888.87	Joback Method
cpg	841.57	J/mol×K	922.49	Joback Method
cpg	853.65	J/mol×K	956.12	Joback Method
cpg	864.77	J/mol×K	989.74	Joback Method
cpg	874.96	J/mol×K	1023.37	Joback Method

Sources

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=U346666&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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