L-Valine, N-(3-fluorobenzoyl)-, dodecyl ester

Inchi: InChI=1S/C24H38FNO3/c1-4-5-6-7-8-9-10-11-12-13-17-29-24(28)22(19(2)3)26-23(27)20
InchiKey: SCXJTQIWHDSOHF-UHFFFAOYSA-N
Formula: C24H38FNO3
SMILES: CCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(F)c1)C(C)C
Mol. weight [g/mol]: 407.56

Physical Properties

Property code	Value	Unit	Source
gf	-219.16	kJ/mol	Joback Method
hf	-824.21	kJ/mol	Joback Method
hfus	57.09	kJ/mol	Joback Method
hvap	92.70	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	6.044		Crippen Method
mcvol	346.020	ml/mol	McGowan Method
pc	1031.91	kPa	Joback Method
rinpol	2826.00		NIST Webbook
rinpol	2826.00		NIST Webbook
tb	958.90	K	Joback Method
tc	1173.99	K	Joback Method
tf	544.52	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1158.56	J/mol×K	958.90	Joback Method
cpg	1175.20	J/mol×K	994.75	Joback Method
cpg	1190.50	J/mol×K	1030.60	Joback Method
cpg	1204.52	J/mol×K	1066.45	Joback Method
cpg	1217.33	J/mol×K	1102.30	Joback Method
cpg	1228.98	J/mol×K	1138.15	Joback Method
cpg	1239.53	J/mol×K	1173.99	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=U346679&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