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

Inchi: InChI=1S/C30H50FNO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-24-35-30(34)28(
InchiKey: FKUIILACOJINNC-UHFFFAOYSA-N
Formula: C30H50FNO3
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1ccc(F)cc1)C(C)C
Mol. weight [g/mol]: 491.72

Physical Properties

Property code	Value	Unit	Source
gf	-168.64	kJ/mol	Joback Method
hf	-948.05	kJ/mol	Joback Method
hfus	72.63	kJ/mol	Joback Method
hvap	106.06	kJ/mol	Joback Method
log10ws	-10.09		Crippen Method
logp	8.385		Crippen Method
mcvol	430.560	ml/mol	McGowan Method
pc	734.82	kPa	Joback Method
rinpol	3459.00		NIST Webbook
rinpol	3459.00		NIST Webbook
tb	1096.18	K	Joback Method
tc	1361.73	K	Joback Method
tf	612.14	K	Joback Method
vc	1.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1536.44	J/mol×K	1096.18	Joback Method
cpg	1555.67	J/mol×K	1140.44	Joback Method
cpg	1572.91	J/mol×K	1184.70	Joback Method
cpg	1588.31	J/mol×K	1228.96	Joback Method
cpg	1602.02	J/mol×K	1273.21	Joback Method
cpg	1614.20	J/mol×K	1317.47	Joback Method
cpg	1624.98	J/mol×K	1361.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346677&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