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

Inchi: InChI=1S/C26H42FNO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-31-26(30)24(21(2)3)28-25
InchiKey: IZHTXRVBUGMZRX-UHFFFAOYSA-N
Formula: C26H42FNO3
SMILES: CCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(F)c1)C(C)C
Mol. weight [g/mol]: 435.62

Physical Properties

Property code	Value	Unit	Source
gf	-202.32	kJ/mol	Joback Method
hf	-865.49	kJ/mol	Joback Method
hfus	62.27	kJ/mol	Joback Method
hvap	97.15	kJ/mol	Joback Method
log10ws	-8.42		Crippen Method
logp	6.824		Crippen Method
mcvol	374.200	ml/mol	McGowan Method
pc	915.50	kPa	Joback Method
rinpol	3047.00		NIST Webbook
rinpol	3047.00		NIST Webbook
tb	1004.66	K	Joback Method
tc	1231.64	K	Joback Method
tf	567.06	K	Joback Method
vc	1.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1282.94	J/mol×K	1004.66	Joback Method
cpg	1300.27	J/mol×K	1042.49	Joback Method
cpg	1316.09	J/mol×K	1080.32	Joback Method
cpg	1330.49	J/mol×K	1118.15	Joback Method
cpg	1343.55	J/mol×K	1155.98	Joback Method
cpg	1355.35	J/mol×K	1193.81	Joback Method
cpg	1365.96	J/mol×K	1231.64	Joback Method

Sources

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=U346680&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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