L-Valine, N-(2-fluoro-3-trifluoromethylbenzoyl)-, hexadecyl ester

Inchi: InChI=1S/C29H45F4NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-37-28(36)26(22(2)
InchiKey: ABPCDLZDXOQOFJ-UHFFFAOYSA-N
Formula: C29H45F4NO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1F)C(C)C
Mol. weight [g/mol]: 531.67

Physical Properties

Property code	Value	Unit	Source
gf	-768.28	kJ/mol	Joback Method
hf	-1535.96	kJ/mol	Joback Method
hfus	71.47	kJ/mol	Joback Method
hvap	100.75	kJ/mol	Joback Method
log10ws	-10.36		Crippen Method
logp	8.623		Crippen Method
mcvol	421.780	ml/mol	McGowan Method
pc	721.08	kPa	Joback Method
rinpol	3150.00		NIST Webbook
rinpol	3150.00		NIST Webbook
tb	1072.86	K	Joback Method
tc	1335.87	K	Joback Method
tf	617.58	K	Joback Method
vc	1.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1491.15	J/mol×K	1072.86	Joback Method
cpg	1510.22	J/mol×K	1116.69	Joback Method
cpg	1527.55	J/mol×K	1160.53	Joback Method
cpg	1543.30	J/mol×K	1204.36	Joback Method
cpg	1557.66	J/mol×K	1248.20	Joback Method
cpg	1570.78	J/mol×K	1292.03	Joback Method
cpg	1582.85	J/mol×K	1335.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346476&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