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

Inchi: InChI=1S/C30H47F4NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-38-29(37)27(23
Inchikey: XUTXJSFAUWAQAZ-UHFFFAOYSA-N
Formula: C30H47F4NO3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1F)C(C)C
Mol. weight [g/mol]: 545.69

Physical Properties

Property code	Value	Unit	Source
gf	-759.86	kJ/mol	Joback Method
hf	-1556.60	kJ/mol	Joback Method
hfus	74.06	kJ/mol	Joback Method
hvap	102.97	kJ/mol	Joback Method
log10ws	-10.77		Crippen Method
logp	9.014		Crippen Method
mcvol	435.870	ml/mol	McGowan Method
pc	685.29	kPa	Joback Method
rinpol	3258.00		NIST Webbook
rinpol	3258.00		NIST Webbook
tb	1095.74	K	Joback Method
tc	1372.53	K	Joback Method
tf	628.85	K	Joback Method
vc	1.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1554.86	J/mol×K	1095.74	Joback Method
cpg	1574.73	J/mol×K	1141.87	Joback Method
cpg	1592.72	J/mol×K	1188.00	Joback Method
cpg	1609.04	J/mol×K	1234.13	Joback Method
cpg	1623.89	J/mol×K	1280.26	Joback Method
cpg	1637.49	J/mol×K	1326.40	Joback Method
cpg	1650.03	J/mol×K	1372.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346477&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