L-Valine, N-(2,5-ditrifluoromethylbenzoyl)-, hexadecyl ester

Inchi: InChI=1S/C30H45F6NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-40-28(39)26(22(2)
InchiKey: XOVFPYVKOAZFEQ-UHFFFAOYSA-N
Formula: C30H45F6NO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F)C(C)C
Mol. weight [g/mol]: 581.67

Physical Properties

Property code	Value	Unit	Source
gf	-1146.64	kJ/mol	Joback Method
hf	-1957.57	kJ/mol	Joback Method
hfus	72.81	kJ/mol	Joback Method
hvap	100.04	kJ/mol	Joback Method
log10ws	-11.13		Crippen Method
logp	9.503		Crippen Method
mcvol	439.410	ml/mol	McGowan Method
pc	660.51	kPa	Joback Method
rinpol	3024.00		NIST Webbook
rinpol	3024.00		NIST Webbook
tb	1091.05	K	Joback Method
tc	1371.49	K	Joback Method
tf	632.45	K	Joback Method
vc	1.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1567.81	J/mol×K	1091.05	Joback Method
cpg	1588.28	J/mol×K	1137.79	Joback Method
cpg	1607.14	J/mol×K	1184.53	Joback Method
cpg	1624.67	J/mol×K	1231.27	Joback Method
cpg	1641.13	J/mol×K	1278.01	Joback Method
cpg	1656.78	J/mol×K	1324.75	Joback Method
cpg	1671.89	J/mol×K	1371.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346580&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