L-Valine, N-(3-trifluoromethylbenzoyl)-, pentadecyl ester

Inchi: InChI=1S/C28H44F3NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-20-35-27(34)25(22(2)3)3

InchiKey: KPFDUOLYSQBMEJ-UHFFFAOYSA-N

Formula: C28H44F3NO3

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1)C(C)C

Mol. weight [g/mol]: 499.65

Physical Properties

Property code	Value	Unit	Source
gf	-572.26	kJ/mol	Joback Method
hf	-1307.74	kJ/mol	Joback Method
hfus	66.19	kJ/mol	Joback Method
hvap	98.67	kJ/mol	Joback Method
log10ws	-9.61		Crippen Method
logp	8.094		Crippen Method
mcvol	405.920	ml/mol	McGowan Method
pc	785.51	kPa	Joback Method
rinpol	3065.00		NIST Webbook
rinpol	3065.00		NIST Webbook
tb	1045.73	K	Joback Method
tc	1290.61	K	Joback Method
tf	593.20	K	Joback Method
vc	1.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1422.02	J/mol×K	1045.73	Joback Method
cpg	1440.35	J/mol×K	1086.54	Joback Method
cpg	1457.16	J/mol×K	1127.36	Joback Method
cpg	1472.59	J/mol×K	1168.17	Joback Method
cpg	1486.79	J/mol×K	1208.98	Joback Method
cpg	1499.88	J/mol×K	1249.80	Joback Method
cpg	1512.02	J/mol×K	1290.61	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=U346727&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