L-Valine, N-(2-trifluoromethylbenzoyl)-, dodecyl ester

Inchi: InChI=1S/C25H38F3NO3/c1-4-5-6-7-8-9-10-11-12-15-18-32-24(31)22(19(2)3)29-23(30)2

InchiKey: JTIJEKZCKRZUSM-UHFFFAOYSA-N

Formula: C25H38F3NO3

SMILES: CCCCCCCCCCCCOC(=O)C(NC(=O)c1ccccc1C(F)(F)F)C(C)C

Mol. weight [g/mol]: 457.57

Physical Properties

Property code	Value	Unit	Source
gf	-597.52	kJ/mol	Joback Method
hf	-1245.82	kJ/mol	Joback Method
hfus	58.42	kJ/mol	Joback Method
hvap	92.00	kJ/mol	Joback Method
log10ws	-8.35		Crippen Method
logp	6.924		Crippen Method
mcvol	363.650	ml/mol	McGowan Method
pc	929.51	kPa	Joback Method
rinpol	2824.00		NIST Webbook
rinpol	2824.00		NIST Webbook
tb	977.09	K	Joback Method
tc	1197.09	K	Joback Method
tf	559.39	K	Joback Method
vc	1.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1234.12	J/mol×K	977.09	Joback Method
cpg	1250.84	J/mol×K	1013.76	Joback Method
cpg	1266.26	J/mol×K	1050.42	Joback Method
cpg	1280.50	J/mol×K	1087.09	Joback Method
cpg	1293.63	J/mol×K	1123.76	Joback Method
cpg	1305.75	J/mol×K	1160.42	Joback Method
cpg	1316.95	J/mol×K	1197.09	Joback Method

Sources

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=U346712&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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