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

Inchi: InChI=1S/C24H36F3NO3/c1-4-5-6-7-8-9-10-11-14-17-31-23(30)21(18(2)3)28-22(29)19-1

InchiKey: HAXJOSUTEMAKIT-UHFFFAOYSA-N

Formula: C24H36F3NO3

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

Mol. weight [g/mol]: 443.54

Physical Properties

Property code	Value	Unit	Source
gf	-605.94	kJ/mol	Joback Method
hf	-1225.18	kJ/mol	Joback Method
hfus	55.83	kJ/mol	Joback Method
hvap	89.77	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	6.534		Crippen Method
mcvol	349.560	ml/mol	McGowan Method
pc	986.40	kPa	Joback Method
rinpol	2734.00		NIST Webbook
rinpol	2734.00		NIST Webbook
tb	954.21	K	Joback Method
tc	1168.26	K	Joback Method
tf	548.12	K	Joback Method
vc	1.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1172.45	J/mol×K	954.21	Joback Method
cpg	1188.74	J/mol×K	989.89	Joback Method
cpg	1203.80	J/mol×K	1025.56	Joback Method
cpg	1217.72	J/mol×K	1061.24	Joback Method
cpg	1230.57	J/mol×K	1096.91	Joback Method
cpg	1242.44	J/mol×K	1132.59	Joback Method
cpg	1253.41	J/mol×K	1168.26	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=U346711&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