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

Inchi: InChI=1S/C24H33F6NO3/c1-4-5-6-7-8-9-10-11-14-34-22(33)20(16(2)3)31-21(32)18-15-1

InchiKey: VVLVCXQDILIRRG-UHFFFAOYSA-N

Formula: C24H33F6NO3

SMILES: CCCCCCCCCCOC(=O)C(NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F)C(C)C

Mol. weight [g/mol]: 497.51

Physical Properties

Property code	Value	Unit	Source
gf	-1197.16	kJ/mol	Joback Method
hf	-1833.73	kJ/mol	Joback Method
hfus	57.27	kJ/mol	Joback Method
hvap	86.69	kJ/mol	Joback Method
log10ws	-8.62		Crippen Method
logp	7.163		Crippen Method
mcvol	354.870	ml/mol	McGowan Method
pc	909.98	kPa	Joback Method
rinpol	2432.00		NIST Webbook
rinpol	2432.00		NIST Webbook
tb	953.77	K	Joback Method
tc	1169.19	K	Joback Method
tf	564.83	K	Joback Method
vc	1.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1192.64	J/mol×K	953.77	Joback Method
cpg	1208.44	J/mol×K	989.67	Joback Method
cpg	1223.09	J/mol×K	1025.58	Joback Method
cpg	1236.69	J/mol×K	1061.48	Joback Method
cpg	1249.34	J/mol×K	1097.39	Joback Method
cpg	1261.15	J/mol×K	1133.29	Joback Method
cpg	1272.20	J/mol×K	1169.19	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=U346575&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