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

Inchi: InChI=1S/C23H34F3NO3/c1-4-5-6-7-8-9-10-13-16-30-22(29)20(17(2)3)27-21(28)18-14-1

InchiKey: JCCQGZJXUHWGBJ-UHFFFAOYSA-N

Formula: C23H34F3NO3

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

Mol. weight [g/mol]: 429.52

Physical Properties

Property code	Value	Unit	Source
gf	-614.36	kJ/mol	Joback Method
hf	-1204.54	kJ/mol	Joback Method
hfus	53.24	kJ/mol	Joback Method
hvap	87.54	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	6.144		Crippen Method
mcvol	335.470	ml/mol	McGowan Method
pc	1048.69	kPa	Joback Method
rinpol	2639.00		NIST Webbook
rinpol	2639.00		NIST Webbook
tb	931.33	K	Joback Method
tc	1140.47	K	Joback Method
tf	536.85	K	Joback Method
vc	1.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1111.33	J/mol×K	931.33	Joback Method
cpg	1127.23	J/mol×K	966.19	Joback Method
cpg	1141.96	J/mol×K	1001.04	Joback Method
cpg	1155.59	J/mol×K	1035.90	Joback Method
cpg	1168.19	J/mol×K	1070.75	Joback Method
cpg	1179.84	J/mol×K	1105.61	Joback Method
cpg	1190.61	J/mol×K	1140.47	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=U346710&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