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

Inchi: InChI=1S/C21H30F3NO3/c1-4-5-6-7-8-11-14-28-20(27)18(15(2)3)25-19(26)16-12-9-10-1

InchiKey: ZCGYWJSYHRKSFK-UHFFFAOYSA-N

Formula: C21H30F3NO3

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

Mol. weight [g/mol]: 401.46

Physical Properties

Property code	Value	Unit	Source
gf	-631.20	kJ/mol	Joback Method
hf	-1163.26	kJ/mol	Joback Method
hfus	48.06	kJ/mol	Joback Method
hvap	83.09	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	5.364		Crippen Method
mcvol	307.290	ml/mol	McGowan Method
pc	1192.35	kPa	Joback Method
rinpol	2440.00		NIST Webbook
rinpol	2440.00		NIST Webbook
tb	885.57	K	Joback Method
tc	1087.70	K	Joback Method
tf	514.31	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	990.90	J/mol×K	885.57	Joback Method
cpg	1006.15	J/mol×K	919.26	Joback Method
cpg	1020.30	J/mol×K	952.95	Joback Method
cpg	1033.42	J/mol×K	986.64	Joback Method
cpg	1045.58	J/mol×K	1020.33	Joback Method
cpg	1056.82	J/mol×K	1054.02	Joback Method
cpg	1067.22	J/mol×K	1087.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346708&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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