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

Inchi: InChI=1S/C21H27F6NO3/c1-4-5-6-7-8-11-31-19(30)17(13(2)3)28-18(29)15-12-14(20(22,
InchiKey: PUYZHODXUKTUER-UHFFFAOYSA-N
Formula: C21H27F6NO3
SMILES: CCCCCCCOC(=O)C(NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F)C(C)C
Mol. weight [g/mol]: 455.43

Physical Properties

Property code	Value	Unit	Source
gf	-1222.42	kJ/mol	Joback Method
hf	-1771.81	kJ/mol	Joback Method
hfus	49.50	kJ/mol	Joback Method
hvap	80.01	kJ/mol	Joback Method
log10ws	-7.36		Crippen Method
logp	5.992		Crippen Method
mcvol	312.600	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
rinpol	2148.00		NIST Webbook
rinpol	2148.00		NIST Webbook
tb	885.13	K	Joback Method
tc	1084.42	K	Joback Method
tf	531.02	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1012.43	J/mol×K	885.13	Joback Method
cpg	1026.81	J/mol×K	918.35	Joback Method
cpg	1040.17	J/mol×K	951.56	Joback Method
cpg	1052.60	J/mol×K	984.78	Joback Method
cpg	1064.15	J/mol×K	1017.99	Joback Method
cpg	1074.91	J/mol×K	1051.21	Joback Method
cpg	1084.94	J/mol×K	1084.42	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=U346573&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