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

Inchi: InChI=1S/C19H26F3NO3/c1-4-5-6-9-12-26-18(25)16(13(2)3)23-17(24)14-10-7-8-11-15(1

InchiKey: UHTDDHOVRBVHBC-UHFFFAOYSA-N

Formula: C19H26F3NO3

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

Mol. weight [g/mol]: 373.41

Physical Properties

Property code	Value	Unit	Source
gf	-648.04	kJ/mol	Joback Method
hf	-1121.98	kJ/mol	Joback Method
hfus	42.88	kJ/mol	Joback Method
hvap	78.64	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	4.583		Crippen Method
mcvol	279.110	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
rinpol	2238.00		NIST Webbook
rinpol	2238.00		NIST Webbook
tb	839.81	K	Joback Method
tc	1038.28	K	Joback Method
tf	491.77	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.23	J/mol×K	839.81	Joback Method
cpg	887.90	J/mol×K	872.89	Joback Method
cpg	901.55	J/mol×K	905.97	Joback Method
cpg	914.22	J/mol×K	939.04	Joback Method
cpg	925.96	J/mol×K	972.12	Joback Method
cpg	936.83	J/mol×K	1005.20	Joback Method
cpg	946.87	J/mol×K	1038.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346706&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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