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

Inchi: InChI=1S/C18H21F6NO3/c1-4-5-8-28-16(27)14(10(2)3)25-15(26)12-9-11(17(19,20)21)6-

InchiKey: PAWHMEAFLYPFBO-UHFFFAOYSA-N

Formula: C18H21F6NO3

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

Mol. weight [g/mol]: 413.35

Physical Properties

Property code	Value	Unit	Source
gf	-1247.68	kJ/mol	Joback Method
hf	-1709.89	kJ/mol	Joback Method
hfus	41.73	kJ/mol	Joback Method
hvap	73.33	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	4.822		Crippen Method
mcvol	270.330	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	1883.00		NIST Webbook
rinpol	1883.00		NIST Webbook
tb	816.49	K	Joback Method
tc	1007.69	K	Joback Method
tf	497.21	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.59	J/mol×K	816.49	Joback Method
cpg	851.85	J/mol×K	848.36	Joback Method
cpg	864.18	J/mol×K	880.22	Joback Method
cpg	875.64	J/mol×K	912.09	Joback Method
cpg	886.29	J/mol×K	943.95	Joback Method
cpg	896.19	J/mol×K	975.82	Joback Method
cpg	905.38	J/mol×K	1007.69	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=U346569&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