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

Inchi: InChI=1S/C17H22F3NO3/c1-4-5-10-24-16(23)14(11(2)3)21-15(22)12-8-6-7-9-13(12)17(1

InchiKey: DJJZASPPJFALHB-UHFFFAOYSA-N

Formula: C17H22F3NO3

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

Mol. weight [g/mol]: 345.36

Physical Properties

Property code	Value	Unit	Source
gf	-664.88	kJ/mol	Joback Method
hf	-1080.70	kJ/mol	Joback Method
hfus	37.70	kJ/mol	Joback Method
hvap	74.19	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	3.803		Crippen Method
mcvol	250.930	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	2049.00		NIST Webbook
rinpol	2049.00		NIST Webbook
tb	794.05	K	Joback Method
tc	991.72	K	Joback Method
tf	469.23	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.76	J/mol×K	794.05	Joback Method
cpg	772.89	J/mol×K	827.00	Joback Method
cpg	786.04	J/mol×K	859.94	Joback Method
cpg	798.24	J/mol×K	892.89	Joback Method
cpg	809.55	J/mol×K	925.83	Joback Method
cpg	820.02	J/mol×K	958.78	Joback Method
cpg	829.68	J/mol×K	991.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346704&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

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