L-Valine, N-(3-fluoro-4-trifluoromethylbenzoyl)-, butyl ester

Inchi: InChI=1S/C17H21F4NO3/c1-4-5-8-25-16(24)14(10(2)3)22-15(23)11-6-7-12(13(18)9-11)17(19,20)21/h6-7,9-10,14H,4-5,8H2,1-3H3,(H,22,23)/t14-/m0/s1

InchiKey: HUOOHLBMNVKAGK-UHFFFAOYSA-N

Formula: C17H21F4NO3

SMILES: CCCCOC(=O)C(NC(=O)c1ccc(C(F)(F)F)c(F)c1)C(C)C

Mol. weight [g/mol]: 363.35

Physical Properties

Property code	Value	Unit	Source
gf	-869.32	kJ/mol	Joback Method
hf	-1288.28	kJ/mol	Joback Method
hfus	40.39	kJ/mol	Joback Method
hvap	74.03	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	3.942		Crippen Method
mcvol	252.700	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	1905.00		NIST Webbook
rinpol	1905.00		NIST Webbook
tb	798.30	K	Joback Method
tc	991.98	K	Joback Method
tf	482.34	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.41	J/mol×K	798.30	Joback Method
cpg	779.02	J/mol×K	830.58	Joback Method
cpg	791.69	J/mol×K	862.86	Joback Method
cpg	803.47	J/mol×K	895.14	Joback Method
cpg	814.39	J/mol×K	927.42	Joback Method
cpg	824.50	J/mol×K	959.70	Joback Method
cpg	833.82	J/mol×K	991.98	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=U346552&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

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