L-Valine, N-(2-fluoro-3-trifluoromethylbenzoyl)-, isobutyl ester

Inchi: InChI=1S/C17H21F4NO3/c1-9(2)8-25-16(24)14(10(3)4)22-15(23)11-6-5-7-12(13(11)18)17(19,20)21/h5-7,9-10,14H,8H2,1-4H3,(H,22,23)/t14-/m0/s1

InchiKey: QYFLAYRTQBNTPP-UHFFFAOYSA-N

Formula: C17H21F4NO3

SMILES: CC(C)COC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1F)C(C)C

Mol. weight [g/mol]: 363.35

Physical Properties

Property code	Value	Unit	Source
gf	-871.76	kJ/mol	Joback Method
hf	-1293.56	kJ/mol	Joback Method
hfus	36.87	kJ/mol	Joback Method
hvap	73.65	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	3.798		Crippen Method
mcvol	252.700	ml/mol	McGowan Method
pc	1521.12	kPa	Joback Method
rinpol	1929.00		NIST Webbook
rinpol	1929.00		NIST Webbook
tb	797.86	K	Joback Method
tc	993.48	K	Joback Method
tf	467.34	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.96	J/mol×K	797.86	Joback Method
cpg	779.71	J/mol×K	830.46	Joback Method
cpg	792.49	J/mol×K	863.07	Joback Method
cpg	804.35	J/mol×K	895.67	Joback Method
cpg	815.32	J/mol×K	928.28	Joback Method
cpg	825.46	J/mol×K	960.88	Joback Method
cpg	834.79	J/mol×K	993.48	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346465&Units=SI

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