«beta»-Alanine, N-(3-fluorobenzoyl)-, butyl ester

Inchi: InChI=1S/C14H18FNO3/c1-2-3-9-19-13(17)7-8-16-14(18)11-5-4-6-12(15)10-11/h4-6,10H

InchiKey: HXHPIJAUAFFOKH-UHFFFAOYSA-N

Formula: C14H18FNO3

SMILES: CCCCOC(=O)CCNC(=O)c1cccc(F)c1

Mol. weight [g/mol]: 267.30

Physical Properties

Property code	Value	Unit	Source
gf	-298.48	kJ/mol	Joback Method
hf	-607.25	kJ/mol	Joback Method
hfus	38.23	kJ/mol	Joback Method
hvap	71.22	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.289		Crippen Method
mcvol	205.120	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	2044.00		NIST Webbook
rinpol	2044.00		NIST Webbook
tb	730.98	K	Joback Method
tc	931.51	K	Joback Method
tf	461.82	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.91	J/mol×K	730.98	Joback Method
cpg	588.47	J/mol×K	764.40	Joback Method
cpg	601.16	J/mol×K	797.82	Joback Method
cpg	612.99	J/mol×K	831.24	Joback Method
cpg	623.99	J/mol×K	864.66	Joback Method
cpg	634.19	J/mol×K	898.08	Joback Method
cpg	643.60	J/mol×K	931.51	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=U321934&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