«beta»-Alanine, N-(2,3,4-trifluorobenzoyl)-, butyl ester

Inchi: InChI=1S/C14H16F3NO3/c1-2-3-8-21-11(19)6-7-18-14(20)9-4-5-10(15)13(17)12(9)16/h4

InchiKey: VUAYIYCGPHNIKY-UHFFFAOYSA-N

Formula: C14H16F3NO3

SMILES: CCCCOC(=O)CCNC(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 303.28

Physical Properties

Property code	Value	Unit	Source
gf	-707.36	kJ/mol	Joback Method
hf	-1022.41	kJ/mol	Joback Method
hfus	43.61	kJ/mol	Joback Method
hvap	70.91	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	2.567		Crippen Method
mcvol	208.660	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	1959.00		NIST Webbook
rinpol	1959.00		NIST Webbook
tb	739.48	K	Joback Method
tc	929.15	K	Joback Method
tf	488.04	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.45	J/mol×K	739.48	Joback Method
cpg	600.82	J/mol×K	771.09	Joback Method
cpg	612.43	J/mol×K	802.70	Joback Method
cpg	623.30	J/mol×K	834.31	Joback Method
cpg	633.44	J/mol×K	865.93	Joback Method
cpg	642.86	J/mol×K	897.54	Joback Method
cpg	651.58	J/mol×K	929.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321691&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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