Phenylglycine, butyl ester, TFA

Inchi: InChI=1S/C14H16F3NO3/c1-2-3-9-21-12(19)11(10-7-5-4-6-8-10)18-13(20)14(15,16)17/h
InchiKey: SNHZNSLGUMXDKP-UHFFFAOYSA-N
Formula: C14H16F3NO3
SMILES: CCCCOC(=O)C(NC(=O)C(F)(F)F)c1ccccc1
Mol. weight [g/mol]: 303.28

Physical Properties

Property code	Value	Unit	Source
gf	-678.07	kJ/mol	Joback Method
hf	-1002.03	kJ/mol	Joback Method
hfus	33.84	kJ/mol	Joback Method
hvap	67.24	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.749		Crippen Method
mcvol	208.660	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
rinpol	1584.00		NIST Webbook
tb	720.87	K	Joback Method
tc	918.04	K	Joback Method
tf	437.90	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.66	J/mol×K	720.87	Joback Method
cpg	607.76	J/mol×K	753.73	Joback Method
cpg	619.95	J/mol×K	786.59	Joback Method
cpg	631.26	J/mol×K	819.45	Joback Method
cpg	641.73	J/mol×K	852.32	Joback Method
cpg	651.42	J/mol×K	885.18	Joback Method
cpg	660.37	J/mol×K	918.04	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=R32044&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