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

Inchi: InChI=1S/C12H12F3NO3/c1-2-19-9(17)5-6-16-12(18)7-3-4-8(13)11(15)10(7)14/h3-4H,2,

InchiKey: GGRSNVJKBJMWCU-UHFFFAOYSA-N

Formula: C12H12F3NO3

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

Mol. weight [g/mol]: 275.22

Physical Properties

Property code	Value	Unit	Source
gf	-724.20	kJ/mol	Joback Method
hf	-981.13	kJ/mol	Joback Method
hfus	38.43	kJ/mol	Joback Method
hvap	66.45	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	1.787		Crippen Method
mcvol	180.480	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	1763.00		NIST Webbook
rinpol	1763.00		NIST Webbook
tb	693.72	K	Joback Method
tc	885.41	K	Joback Method
tf	465.50	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.62	J/mol×K	693.72	Joback Method
cpg	494.95	J/mol×K	725.67	Joback Method
cpg	505.61	J/mol×K	757.62	Joback Method
cpg	515.61	J/mol×K	789.57	Joback Method
cpg	524.95	J/mol×K	821.51	Joback Method
cpg	533.65	J/mol×K	853.46	Joback Method
cpg	541.70	J/mol×K	885.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321688&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

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