«beta»-Alanine, N-(4-trifluoromethylbenzoyl)-, propyl ester

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

InchiKey: FLZAOZKNARYWDO-UHFFFAOYSA-N

Formula: C14H16F3NO3

SMILES: CCCOC(=O)CCNC(=O)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 303.28

Physical Properties

Property code	Value	Unit	Source
gf	-685.26	kJ/mol	Joback Method
hf	-1008.22	kJ/mol	Joback Method
hfus	36.98	kJ/mol	Joback Method
hvap	68.29	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	2.778		Crippen Method
mcvol	208.660	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	1921.00		NIST Webbook
rinpol	1921.00		NIST Webbook
tb	726.29	K	Joback Method
tc	921.44	K	Joback Method
tf	465.42	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.07	J/mol×K	726.29	Joback Method
cpg	605.84	J/mol×K	758.82	Joback Method
cpg	617.75	J/mol×K	791.34	Joback Method
cpg	628.84	J/mol×K	823.87	Joback Method
cpg	639.14	J/mol×K	856.39	Joback Method
cpg	648.68	J/mol×K	888.92	Joback Method
cpg	657.52	J/mol×K	921.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321738&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