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

Inchi: InChI=1S/C13H14F3NO3/c1-2-7-20-10(18)5-6-17-13(19)8-3-4-9(14)12(16)11(8)15/h3-4H
InchiKey: NQMCWLSODNIJLE-UHFFFAOYSA-N
Formula: C13H14F3NO3
SMILES: CCCOC(=O)CCNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 289.25

Physical Properties

Property code	Value	Unit	Source
gf	-715.78	kJ/mol	Joback Method
hf	-1001.77	kJ/mol	Joback Method
hfus	41.02	kJ/mol	Joback Method
hvap	68.68	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	2.177		Crippen Method
mcvol	194.570	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	1855.00		NIST Webbook
rinpol	1855.00		NIST Webbook
tb	716.60	K	Joback Method
tc	907.04	K	Joback Method
tf	476.77	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.42	J/mol×K	716.60	Joback Method
cpg	547.29	J/mol×K	748.34	Joback Method
cpg	558.45	J/mol×K	780.08	Joback Method
cpg	568.92	J/mol×K	811.82	Joback Method
cpg	578.68	J/mol×K	843.56	Joback Method
cpg	587.77	J/mol×K	875.30	Joback Method
cpg	596.17	J/mol×K	907.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321689&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