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

Inchi: InChI=1S/C13H16FNO3/c1-2-9-18-12(16)7-8-15-13(17)10-3-5-11(14)6-4-10/h3-6H,2,7-9

InchiKey: IMXAWXOVWAWUON-UHFFFAOYSA-N

Formula: C13H16FNO3

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

Mol. weight [g/mol]: 253.27

Physical Properties

Property code	Value	Unit	Source
gf	-306.90	kJ/mol	Joback Method
hf	-586.61	kJ/mol	Joback Method
hfus	35.64	kJ/mol	Joback Method
hvap	68.99	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	1.899		Crippen Method
mcvol	191.030	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1958.00		NIST Webbook
tb	708.10	K	Joback Method
tc	910.62	K	Joback Method
tf	450.55	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.81	J/mol×K	708.10	Joback Method
cpg	534.94	J/mol×K	741.85	Joback Method
cpg	547.22	J/mol×K	775.61	Joback Method
cpg	558.68	J/mol×K	809.36	Joback Method
cpg	569.34	J/mol×K	843.11	Joback Method
cpg	579.22	J/mol×K	876.87	Joback Method
cpg	588.34	J/mol×K	910.62	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=U321755&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