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

Inchi: InChI=1S/C12H14FNO3/c1-2-17-11(15)7-8-14-12(16)9-3-5-10(13)6-4-9/h3-6H,2,7-8H2,1

InchiKey: QKUDTVCOXZRHAZ-UHFFFAOYSA-N

Formula: C12H14FNO3

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

Mol. weight [g/mol]: 239.24

Physical Properties

Property code	Value	Unit	Source
gf	-315.32	kJ/mol	Joback Method
hf	-565.97	kJ/mol	Joback Method
hfus	33.05	kJ/mol	Joback Method
hvap	66.77	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	1.509		Crippen Method
mcvol	176.940	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
rinpol	1855.00		NIST Webbook
rinpol	1855.00		NIST Webbook
tb	685.22	K	Joback Method
tc	890.17	K	Joback Method
tf	439.28	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.95	J/mol×K	685.22	Joback Method
cpg	482.58	J/mol×K	719.38	Joback Method
cpg	494.40	J/mol×K	753.54	Joback Method
cpg	505.43	J/mol×K	787.70	Joback Method
cpg	515.69	J/mol×K	821.86	Joback Method
cpg	525.19	J/mol×K	856.01	Joback Method
cpg	533.96	J/mol×K	890.17	Joback Method

Sources

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=U321754&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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