«beta»-Alanine, N-(3-fluorobenzoyl)-, pentyl ester

Inchi: InChI=1S/C15H20FNO3/c1-2-3-4-10-20-14(18)8-9-17-15(19)12-6-5-7-13(16)11-12/h5-7,1

InchiKey: SYIXGCNYBMGTIP-UHFFFAOYSA-N

Formula: C15H20FNO3

SMILES: CCCCCOC(=O)CCNC(=O)c1cccc(F)c1

Mol. weight [g/mol]: 281.32

Physical Properties

Property code	Value	Unit	Source
gf	-290.06	kJ/mol	Joback Method
hf	-627.89	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	73.44	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	2.679		Crippen Method
mcvol	219.210	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	2137.00		NIST Webbook
tb	753.86	K	Joback Method
tc	952.88	K	Joback Method
tf	473.09	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.18	J/mol×K	753.86	Joback Method
cpg	643.12	J/mol×K	787.03	Joback Method
cpg	656.15	J/mol×K	820.20	Joback Method
cpg	668.31	J/mol×K	853.37	Joback Method
cpg	679.60	J/mol×K	886.54	Joback Method
cpg	690.07	J/mol×K	919.71	Joback Method
cpg	699.74	J/mol×K	952.88	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=U321935&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