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

Inchi: InChI=1S/C17H24FNO3/c1-2-3-4-5-6-12-22-16(20)10-11-19-17(21)14-8-7-9-15(18)13-14

InchiKey: HBICTNOIJPGLBT-UHFFFAOYSA-N

Formula: C17H24FNO3

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

Mol. weight [g/mol]: 309.38

Physical Properties

Property code	Value	Unit	Source
gf	-273.22	kJ/mol	Joback Method
hf	-669.17	kJ/mol	Joback Method
hfus	46.00	kJ/mol	Joback Method
hvap	77.90	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.459		Crippen Method
mcvol	247.390	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	2343.00		NIST Webbook
tb	799.62	K	Joback Method
tc	997.25	K	Joback Method
tf	495.63	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.88	J/mol×K	799.62	Joback Method
cpg	755.47	J/mol×K	832.56	Joback Method
cpg	769.09	J/mol×K	865.50	Joback Method
cpg	781.78	J/mol×K	898.44	Joback Method
cpg	793.56	J/mol×K	931.37	Joback Method
cpg	804.46	J/mol×K	964.31	Joback Method
cpg	814.51	J/mol×K	997.25	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=U321937&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