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

Inchi: InChI=1S/C21H32FNO3/c1-2-3-4-5-6-7-8-9-10-17-26-20(24)15-16-23-21(25)18-11-13-19

InchiKey: UJGFNNWYADAEAC-UHFFFAOYSA-N

Formula: C21H32FNO3

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

Mol. weight [g/mol]: 365.48

Physical Properties

Property code	Value	Unit	Source
gf	-239.54	kJ/mol	Joback Method
hf	-751.73	kJ/mol	Joback Method
hfus	56.36	kJ/mol	Joback Method
hvap	86.80	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.020		Crippen Method
mcvol	303.750	ml/mol	McGowan Method
pc	1238.96	kPa	Joback Method
rinpol	2787.00		NIST Webbook
rinpol	2787.00		NIST Webbook
tb	891.14	K	Joback Method
tc	1093.94	K	Joback Method
tf	540.71	K	Joback Method
vc	1.187	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.93	J/mol×K	891.14	Joback Method
cpg	990.67	J/mol×K	924.94	Joback Method
cpg	1005.29	J/mol×K	958.74	Joback Method
cpg	1018.83	J/mol×K	992.54	Joback Method
cpg	1031.32	J/mol×K	1026.34	Joback Method
cpg	1042.81	J/mol×K	1060.14	Joback Method
cpg	1053.35	J/mol×K	1093.94	Joback Method

Sources

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=U321763&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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