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

Inchi: InChI=1S/C22H34FNO3/c1-2-3-4-5-6-7-8-9-10-11-18-27-21(25)16-17-24-22(26)19-12-14

InchiKey: HDLNWVOAKCQQIB-UHFFFAOYSA-N

Formula: C22H34FNO3

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

Mol. weight [g/mol]: 379.51

Physical Properties

Property code	Value	Unit	Source
gf	-231.12	kJ/mol	Joback Method
hf	-772.37	kJ/mol	Joback Method
hfus	58.95	kJ/mol	Joback Method
hvap	89.02	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.410		Crippen Method
mcvol	317.840	ml/mol	McGowan Method
pc	1159.29	kPa	Joback Method
rinpol	2927.00		NIST Webbook
rinpol	2927.00		NIST Webbook
tb	914.02	K	Joback Method
tc	1120.08	K	Joback Method
tf	551.98	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1035.27	J/mol×K	914.02	Joback Method
cpg	1051.33	J/mol×K	948.36	Joback Method
cpg	1066.21	J/mol×K	982.71	Joback Method
cpg	1079.95	J/mol×K	1017.05	Joback Method
cpg	1092.60	J/mol×K	1051.40	Joback Method
cpg	1104.22	J/mol×K	1085.74	Joback Method
cpg	1114.84	J/mol×K	1120.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321764&Units=SI
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

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