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

Inchi: InChI=1S/C25H40FNO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-20-30-24(28)18-19-27-25(29

InchiKey: FAXNTBJKMVVXAL-UHFFFAOYSA-N

Formula: C25H40FNO3

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

Mol. weight [g/mol]: 421.59

Physical Properties

Property code	Value	Unit	Source
gf	-205.86	kJ/mol	Joback Method
hf	-834.29	kJ/mol	Joback Method
hfus	66.72	kJ/mol	Joback Method
hvap	95.70	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	6.580		Crippen Method
mcvol	360.110	ml/mol	McGowan Method
pc	961.48	kPa	Joback Method
rinpol	3432.00		NIST Webbook
rinpol	3432.00		NIST Webbook
tb	982.66	K	Joback Method
tc	1204.27	K	Joback Method
tf	585.79	K	Joback Method
vc	1.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1219.80	J/mol×K	982.66	Joback Method
cpg	1236.96	J/mol×K	1019.60	Joback Method
cpg	1252.72	J/mol×K	1056.53	Joback Method
cpg	1267.15	J/mol×K	1093.47	Joback Method
cpg	1280.31	J/mol×K	1130.40	Joback Method
cpg	1292.29	J/mol×K	1167.34	Joback Method
cpg	1303.15	J/mol×K	1204.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321943&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