«beta»-Alanine, N-(2,3,4-trifluorobenzoyl)-, pentadecyl ester

Inchi: InChI=1S/C25H38F3NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-19-32-22(30)17-18-29-25(3

InchiKey: DFRQZCCRJJDREW-UHFFFAOYSA-N

Formula: C25H38F3NO3

SMILES: CCCCCCCCCCCCCCCOC(=O)CCNC(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 457.57

Physical Properties

Property code	Value	Unit	Source
gf	-614.74	kJ/mol	Joback Method
hf	-1249.45	kJ/mol	Joback Method
hfus	72.11	kJ/mol	Joback Method
hvap	95.39	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	6.858		Crippen Method
mcvol	363.650	ml/mol	McGowan Method
pc	893.73	kPa	Joback Method
rinpol	3255.00		NIST Webbook
tb	991.16	K	Joback Method
tc	1219.42	K	Joback Method
tf	612.01	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1232.01	J/mol×K	991.16	Joback Method
cpg	1248.99	J/mol×K	1029.20	Joback Method
cpg	1264.44	J/mol×K	1067.25	Joback Method
cpg	1278.44	J/mol×K	1105.29	Joback Method
cpg	1291.05	J/mol×K	1143.33	Joback Method
cpg	1302.33	J/mol×K	1181.38	Joback Method
cpg	1312.35	J/mol×K	1219.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321701&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

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