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

Inchi: InChI=1S/C21H30F3NO3/c1-2-3-4-5-6-7-8-9-10-15-28-18(26)13-14-25-21(27)16-11-12-1

InchiKey: BHVIYNPVUKSNSL-UHFFFAOYSA-N

Formula: C21H30F3NO3

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

Mol. weight [g/mol]: 401.46

Physical Properties

Property code	Value	Unit	Source
gf	-648.42	kJ/mol	Joback Method
hf	-1166.89	kJ/mol	Joback Method
hfus	61.75	kJ/mol	Joback Method
hvap	86.49	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	5.298		Crippen Method
mcvol	307.290	ml/mol	McGowan Method
pc	1140.57	kPa	Joback Method
rinpol	2663.00		NIST Webbook
tb	899.64	K	Joback Method
tc	1101.62	K	Joback Method
tf	566.93	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	987.81	J/mol×K	899.64	Joback Method
cpg	1002.98	J/mol×K	933.30	Joback Method
cpg	1017.01	J/mol×K	966.97	Joback Method
cpg	1029.96	J/mol×K	1000.63	Joback Method
cpg	1041.86	J/mol×K	1034.29	Joback Method
cpg	1052.73	J/mol×K	1067.96	Joback Method
cpg	1062.61	J/mol×K	1101.62	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=U321698&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