«beta»-Alanine, N-(3-trifluoromethylbenzoyl)-, undecyl ester

Inchi: InChI=1S/C22H32F3NO3/c1-2-3-4-5-6-7-8-9-10-16-29-20(27)14-15-26-21(28)18-12-11-1

InchiKey: YVHOANIZTZSQHA-UHFFFAOYSA-N

Formula: C22H32F3NO3

SMILES: CCCCCCCCCCCOC(=O)CCNC(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 415.49

Physical Properties

Property code	Value	Unit	Source
gf	-617.90	kJ/mol	Joback Method
hf	-1173.34	kJ/mol	Joback Method
hfus	57.70	kJ/mol	Joback Method
hvap	86.09	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	5.899		Crippen Method
mcvol	321.380	ml/mol	McGowan Method
pc	1105.21	kPa	Joback Method
rinpol	2743.00		NIST Webbook
rinpol	2743.00		NIST Webbook
tb	909.33	K	Joback Method
tc	1113.71	K	Joback Method
tf	555.58	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1049.85	J/mol×K	909.33	Joback Method
cpg	1065.41	J/mol×K	943.39	Joback Method
cpg	1079.87	J/mol×K	977.46	Joback Method
cpg	1093.30	J/mol×K	1011.52	Joback Method
cpg	1105.77	J/mol×K	1045.58	Joback Method
cpg	1117.33	J/mol×K	1079.65	Joback Method
cpg	1128.06	J/mol×K	1113.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321594&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