«beta»-Alanine, N-(4-trifluoromethylbenzoyl)-, tetradecyl ester

Inchi: InChI=1S/C25H38F3NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-20-32-23(30)18-19-29-24(31)2

InchiKey: TURHBTNXJGAGRL-UHFFFAOYSA-N

Formula: C25H38F3NO3

SMILES: CCCCCCCCCCCCCCOC(=O)CCNC(=O)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 457.57

Physical Properties

Property code	Value	Unit	Source
gf	-592.64	kJ/mol	Joback Method
hf	-1235.26	kJ/mol	Joback Method
hfus	65.47	kJ/mol	Joback Method
hvap	92.77	kJ/mol	Joback Method
log10ws	-8.48		Crippen Method
logp	7.070		Crippen Method
mcvol	363.650	ml/mol	McGowan Method
pc	920.50	kPa	Joback Method
rinpol	3147.00		NIST Webbook
tb	977.97	K	Joback Method
tc	1199.52	K	Joback Method
tf	589.39	K	Joback Method
vc	1.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1233.38	J/mol×K	977.97	Joback Method
cpg	1250.32	J/mol×K	1014.90	Joback Method
cpg	1265.98	J/mol×K	1051.82	Joback Method
cpg	1280.46	J/mol×K	1088.75	Joback Method
cpg	1293.86	J/mol×K	1125.67	Joback Method
cpg	1306.26	J/mol×K	1162.60	Joback Method
cpg	1317.76	J/mol×K	1199.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321747&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