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

Inchi: InChI=1S/C24H36F3NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-31-21(29)16-17-28-24(30)1

InchiKey: HZLZRITZTFPLQW-UHFFFAOYSA-N

Formula: C24H36F3NO3

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

Mol. weight [g/mol]: 443.54

Physical Properties

Property code	Value	Unit	Source
gf	-623.16	kJ/mol	Joback Method
hf	-1228.81	kJ/mol	Joback Method
hfus	69.52	kJ/mol	Joback Method
hvap	93.17	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	6.468		Crippen Method
mcvol	349.560	ml/mol	McGowan Method
pc	947.33	kPa	Joback Method
rinpol	3065.00		NIST Webbook
rinpol	3065.00		NIST Webbook
tb	968.28	K	Joback Method
tc	1188.30	K	Joback Method
tf	600.74	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1170.17	J/mol×K	968.28	Joback Method
cpg	1186.65	J/mol×K	1004.95	Joback Method
cpg	1201.72	J/mol×K	1041.62	Joback Method
cpg	1215.45	J/mol×K	1078.29	Joback Method
cpg	1227.90	J/mol×K	1114.96	Joback Method
cpg	1239.10	J/mol×K	1151.63	Joback Method
cpg	1249.11	J/mol×K	1188.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321700&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