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

Inchi: InChI=1S/C26H40F3NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20-33-23(31)18-19-30-2

InchiKey: UWHRJZOHRBFUBE-UHFFFAOYSA-N

Formula: C26H40F3NO3

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

Mol. weight [g/mol]: 471.60

Physical Properties

Property code	Value	Unit	Source
gf	-606.32	kJ/mol	Joback Method
hf	-1270.09	kJ/mol	Joback Method
hfus	74.70	kJ/mol	Joback Method
hvap	97.62	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	7.248		Crippen Method
mcvol	377.740	ml/mol	McGowan Method
pc	844.56	kPa	Joback Method
rinpol	3483.00		NIST Webbook
rinpol	3483.00		NIST Webbook
tb	1014.04	K	Joback Method
tc	1251.80	K	Joback Method
tf	623.28	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1294.30	J/mol×K	1014.04	Joback Method
cpg	1311.81	J/mol×K	1053.67	Joback Method
cpg	1327.66	J/mol×K	1093.29	Joback Method
cpg	1341.93	J/mol×K	1132.92	Joback Method
cpg	1354.70	J/mol×K	1172.55	Joback Method
cpg	1366.04	J/mol×K	1212.17	Joback Method
cpg	1376.03	J/mol×K	1251.80	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=U321702&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