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

Inchi: InChI=1S/C22H32F3NO3/c1-2-3-4-5-6-7-8-9-10-11-16-29-19(27)14-15-26-22(28)17-12-1

InchiKey: PAWDLTABFBISKR-UHFFFAOYSA-N

Formula: C22H32F3NO3

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

Mol. weight [g/mol]: 415.49

Physical Properties

Property code	Value	Unit	Source
gf	-640.00	kJ/mol	Joback Method
hf	-1187.53	kJ/mol	Joback Method
hfus	64.34	kJ/mol	Joback Method
hvap	88.72	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	5.688		Crippen Method
mcvol	321.380	ml/mol	McGowan Method
pc	1070.06	kPa	Joback Method
rinpol	2776.00		NIST Webbook
tb	922.52	K	Joback Method
tc	1129.48	K	Joback Method
tf	578.20	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.02	J/mol×K	922.52	Joback Method
cpg	1063.59	J/mol×K	957.01	Joback Method
cpg	1077.96	J/mol×K	991.51	Joback Method
cpg	1091.17	J/mol×K	1026.00	Joback Method
cpg	1103.26	J/mol×K	1060.49	Joback Method
cpg	1114.25	J/mol×K	1094.99	Joback Method
cpg	1124.20	J/mol×K	1129.48	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=U321699&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