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

Inchi: InChI=1S/C16H20F3NO3/c1-10(2)4-3-9-23-13(21)7-8-20-16(22)11-5-6-12(17)15(19)14(1

InchiKey: YXHSSAQMISUBOH-UHFFFAOYSA-N

Formula: C16H20F3NO3

SMILES: CC(C)CCCOC(=O)CCNC(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 331.33

Physical Properties

Property code	Value	Unit	Source
gf	-692.96	kJ/mol	Joback Method
hf	-1068.97	kJ/mol	Joback Method
hfus	45.27	kJ/mol	Joback Method
hvap	74.97	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.203		Crippen Method
mcvol	236.840	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	2108.00		NIST Webbook
rinpol	2108.00		NIST Webbook
tb	784.80	K	Joback Method
tc	976.41	K	Joback Method
tf	495.58	K	Joback Method
vc	0.936	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.49	J/mol×K	784.80	Joback Method
cpg	711.85	J/mol×K	816.73	Joback Method
cpg	724.34	J/mol×K	848.67	Joback Method
cpg	735.99	J/mol×K	880.60	Joback Method
cpg	746.81	J/mol×K	912.54	Joback Method
cpg	756.81	J/mol×K	944.47	Joback Method
cpg	766.02	J/mol×K	976.41	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=U321692&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