«beta»-Alanine, N-(3-trifluoromethylbenzoyl)-, hexyl ester

Inchi: InChI=1S/C17H22F3NO3/c1-2-3-4-5-11-24-15(22)9-10-21-16(23)13-7-6-8-14(12-13)17(1

InchiKey: TYUNJHLHZXEUIK-UHFFFAOYSA-N

Formula: C17H22F3NO3

SMILES: CCCCCCOC(=O)CCNC(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 345.36

Physical Properties

Property code	Value	Unit	Source
gf	-660.00	kJ/mol	Joback Method
hf	-1070.14	kJ/mol	Joback Method
hfus	44.75	kJ/mol	Joback Method
hvap	74.97	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	3.949		Crippen Method
mcvol	250.930	ml/mol	McGowan Method
pc	1564.75	kPa	Joback Method
rinpol	2225.00		NIST Webbook
rinpol	2225.00		NIST Webbook
tb	794.93	K	Joback Method
tc	988.51	K	Joback Method
tf	499.23	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.65	J/mol×K	794.93	Joback Method
cpg	771.49	J/mol×K	827.19	Joback Method
cpg	784.40	J/mol×K	859.46	Joback Method
cpg	796.43	J/mol×K	891.72	Joback Method
cpg	807.62	J/mol×K	923.98	Joback Method
cpg	818.01	J/mol×K	956.24	Joback Method
cpg	827.66	J/mol×K	988.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321589&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