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

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

InchiKey: BTJASVJUORKKEC-UHFFFAOYSA-N

Formula: C17H22F3NO3

SMILES: CC(C)CCCOC(=O)CCNC(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 345.36

Physical Properties

Property code	Value	Unit	Source
gf	-662.44	kJ/mol	Joback Method
hf	-1075.42	kJ/mol	Joback Method
hfus	41.23	kJ/mol	Joback Method
hvap	74.58	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	3.805		Crippen Method
mcvol	250.930	ml/mol	McGowan Method
pc	1574.70	kPa	Joback Method
rinpol	2174.00		NIST Webbook
tb	794.49	K	Joback Method
tc	990.05	K	Joback Method
tf	484.23	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.21	J/mol×K	794.49	Joback Method
cpg	772.19	J/mol×K	827.08	Joback Method
cpg	785.21	J/mol×K	859.68	Joback Method
cpg	797.32	J/mol×K	892.27	Joback Method
cpg	808.57	J/mol×K	924.86	Joback Method
cpg	819.00	J/mol×K	957.45	Joback Method
cpg	828.65	J/mol×K	990.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321588&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

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